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Conditionally positive definite kernels: theoritical contribution, application to interpolation and approximation

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Abstract: Since Aronszajn (1950), it is well known that a functional Hilbert space, called Reproducing Kernel Hilbert Space (R.K.H.S), can be associated to any positive definite kernel K. This correspondance is the basis of many useful algorithms. In the more general context of conditionally positive definite kernels the *native spaces* are the usual theoretical framework. However, the definition of *conditionally positive definite* used in that framework is not adapted to extend the results of the positive definite case. We propose a more natural and general definition from which we state a full generalization of Aronszajn's theorem. It states that for every couple $(K, \mathbb{P})$ such that $\mathbb{P}$ is a finite-dimensional vector space of functions and K is a $\mathbb{P}$-conditionally definite positive kernel, there is a unique functional semi-Hilbert space of functions $\mathcal{H}_{K,\mathbb{P}}$ satisfying a generalized reproducing property.
Eventually, we verify that this tool, as native spaces, leads to the same interpolation operator than the one provided by the kriging method and that, using *representer theorem*, we can identify the solution of a regularized regression problem in $\mathcal{H}_{K,\mathbb{P}}$.

Key-words: (Conditionally) Positive Definite Kernel, R.K.H.S, Native Space, Interpolation, Kriging, Regularized Regression

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Noyaux conditionnellement définis positifs : contribution théorique, application à l'interpolation et à l'approximation

Résumé : Il est bien connu, depuis Aronszajn (1950), qu'à tout noyau défini positif K, on peut associer un espace de Hilbert de fonctions, appelé espace de Hilbert à noyau reproduisant associé à K (R.K.H.S). Dans le cas plus général des noyaux conditionnellement positifs, le cadre théorique habituellement invoqué sont les *espaces natifs*. Cependant, la définition de *conditionnellement defini positif* qui y est proposée est trop restrictive pour généraliser complétement le cas défini positif. Nous proposons une définition à la fois plus naturelle et plus générale grâce à laquelle une véritable généralisation du théorème d'Aronszajn est démontrée. En substance, il établit qu'à chaque couple $(K, \mathbb{P})$ tel que $\mathbb{P}$ est un espace vectoriel de fonctions de dimension finie et K est un noyau $\mathbb{P}$-conditionnellement défini positif, il existe un unique espace semi-Hilbertien de fonctions $\mathcal{H}_{K,\mathbb{P}}$ (R.K.S.H.S) satisfaisant une propriété de reproduction généralisée.
Nous vérifions que cet outil, comme les espaces natifs, conduit au même opérateur d'interpolation que la méthode du krigeage et que, utilisant *le théorème du représentant*, on peut identifier la solution d'un problème de régression régularisée dans un R.K.S.H.S .

Mots-clés : Noyau (conditionnellement) défini positif, R.K.H.S , espace natif, interpolation, krigeage, régression régularisée

1 Introduction

Conditionally positive definite kernels arise in many contexts including approximation function algorithms ([9]), surface reconstruction ([11],[6]), numerical analysis of fluid-structure interactions ([10]), computer experiment ([4],[7]), geostatistics ([2], [8]). They are intended to generalize the well known positive definite kernel case. As far as we know, the current mostly used and refered to theoretical framework in conditionally positive definite kernel context, is the *native spaces* theory which was firstly developed by R. Schaback [5] and more recently by H. Wendland [11].

In our opinion, conditionally positive definite kernel definition in the native spaces theory as given in [5] and [11] is not the natural generalization of the positive definite one. We think that the word *definite* in "conditionally positive definite" has not been interpreted in its full genuine meaning by these authors (see below the first remark following Aronszajn's theorem). As a result, the native space theory does not fully contain the positive definite case: for example, it rules out positive definite kernels defining a finite dimensional reproducing kernel Hilbert space. Moreover, the geometrical simplicity of the positive definite case is lost.

In this paper, we first aim at giving general theoretical foundations to conditionally positive definite kernels used to interpolate or to approximate functions. We want these foundations to fully contain the positive definite case.
In the positive definite kernel case the key property is Aronszajn's theorem, which we recall here.
Let $K : E \times E \mapsto \mathbb{R}$ be a positive definite kernel: that is K is symmetric and satisfies the following property

$$\forall (\lambda_1, \mathbf{x}_1) \dots (\lambda_N, \mathbf{x}_N) \in \mathbb{R} \times E, \sum_{1 \le l,m \le N} \lambda_l \lambda_m K(\mathbf{x}_l, \mathbf{x}_m) \ge 0\,.$$

For any $\mathbf{x} \in E$ let us denote by $K_{\mathbf{x}}$ the partial function $\mathbf{x}' \in E \mapsto K(\mathbf{x}, \mathbf{x}') \in \mathbb{R}$.
Let $\mathcal{F}_K$ be the vector space of (finite) linear combinations of functions taken in $\{K_{\mathbf{x}}, \mathbf{x} \in E\}$.
It is easy to see that the formula

$$< \sum_{k=1}^{L} \lambda_l K_{\mathbf{x}_l}, \sum_{m=1}^{M} \mu_m K_{\mathbf{x}'_m} >_{\mathcal{F}_K} = \sum \sum \lambda_l \mu_m K(\mathbf{x}_l, \mathbf{x}'_m)$$

defines a symmetric, positive, bilinear form on $\mathcal{F}_K$. Now Aronszajn's theorem [1] reads as

Theorem 1.1 (Aronszajn) *1. $<,>_{\mathcal{F}_K}$, as a bilinear form, is positive* **definite**.

2. *There is a unique Hilbert space of real functions defined on E, $\mathcal{H}_K$, called Reproducing Kernel Hilbert Space (R.K.H.S) of kernel K such that*
   - *$(\mathcal{F}_K, <,>_{\mathcal{F}_K})$ is a prehilbertian subspace of $\mathcal{H}_K$,*
   - *the following reproducing property is satisfied*

$$\forall f \in \mathcal{H}_K,\ \mathbf{x} \in E,\ f(\mathbf{x}) = < f, K_{\mathbf{x}} >_{\mathcal{H}_K}\,. \qquad (1.1)$$

Let us make several remarks, in the light of that theorem.
First of all, the word *definite* in *positive definite kernels* relates to the positive definiteness of $<,>_{\mathcal{F}_K}$, as stated by point 1 of Theorem 1.1, and not to the positive definiteness of matrices

$$(K(\mathbf{x}_l, \mathbf{x}_m))_{1\leq l,m\leq N}, N \in \mathbb{N}, (\mathbf{x}_1, \ldots, \mathbf{x}_N) \in E^N$$

which are not definite in general.
Secondly, let $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset E$ be a set of points, the reproducing property (1.1), leads to a simple and useful charaterization of the orthogonal projection $S_{K,\mathbf{X}}(f)$ of any $f \in \mathcal{H}_K$ on $\mathcal{F}_K(\mathbf{X})$, the subspace of $\mathcal{F}_K$ spanned by $K_{\mathbf{x}_1}, \ldots, K_{\mathbf{x}_N}$: it is the interpolation of f at the points of $\mathbf{X}$ with minimal $\mathcal{H}_K$-norm.
At last, as an easy consequence of the previous fact, the well known *representer theorem* [3] applied here in a regularized regression context, is stated as follows: let $(\mathbf{x}_1, \mathbf{y}_1), \ldots, (\mathbf{x}_N, \mathbf{y}_N) \in E \times \mathbb{R}$ and $\lambda > 0$,
any solution of

$$\min_{f\in\mathcal{H}_K} \sum_{k=1}^{N} (\mathbf{y}_k - f(\mathbf{x}_k))^2 + \lambda ||f||_{\mathcal{H}_K}$$

lies in $\mathcal{F}_K(\mathbf{X})$.

The main result of our work has exactly the same form as Aronszajn's theorem:

- K, instead of being positive definite, will be what we will call, after a detailed justification, $\mathbb{P}$-conditionally positive definite, where $\mathbb{P}$ is a finite-dimensional vector space of real functions defined on E.
- The R.K.H.S $\mathcal{H}_K$ will be replaced by a $\mathbb{P}$-dependent semi-Hilbert space of functions, satisfying a generalized reproducing property and leading to the acronym ($\mathbb{P}$-)R.K.S.H.S .
- Aronszajn's theorem is recovered for $\mathbb{P} = \{0\}$.

This paper is organised as follows. Section 2 introduces the mathematical objects and notations we need. Section 3 details the relations between these objects leading to a summing up, simple commutative diagram. Section 4 is the core of the paper. There we formulate "our" conditionally positive definite definition, state and prove Aronszajn's theorem analog for conditionally positive definite context. Sections 5 and 6 are devoted to applications. We first state and prove a generalized interpolation result in the spirit of the second remark following Aronszajn's theorem and the useful Lagrange formulation of these interpolations. Besides, we revisit the regularized regression problem in the context of our conditionally positive definite kernels: the representer theorem is verified and an explicit solution of the regularized regression problem is given.

2 First definitions and notation

In this paper, we will denote by

- E an arbitrary set and $\mathbb{R}^E$ the vector space of real functions defined on E

- $\mathbb{P} \subset \mathbb{R}^E$ a n dimensional vector space
- $K : E \times E \mapsto \mathbb{R}$, our generic *kernel*, which is assumed to be, at least, symmetric and $\mathbb{P}$-conditionally positive:

Definition 2.1 ($\mathbb{P}$-conditionally positive kernel) *The kernel K is $\mathbb{P}$-conditionally positive if the following property is satisfied:*

$$\sum_{1 \le k,l \le L} \lambda_l \lambda_k K(\mathbf{x}_l, \mathbf{x}_k) \ge 0$$

for all $L \in \mathbb{N}$, $\mathbf{x}_1, \ldots, \mathbf{x}_L \in E$, $\lambda_1, \ldots, \lambda_L \in \mathbb{R}$ such that

$$\forall p \in \mathbb{P}, \sum_{l=1}^{L} \lambda_l p(\mathbf{x}_l) = 0$$

- $K_{\mathbf{x}}$, for $\mathbf{x} \in E$, the partial function $\mathbf{x}' \in E \mapsto K(\mathbf{x}, \mathbf{x}')$.

2.1 Measures with finite support

Let us set:

- $\delta_{\mathbf{x}}$ the Dirac measure concentrated at $\mathbf{x}$, for any $\mathbf{x} \in E$
- $\mathcal{M}$ the set of real measures on E with finite support:

$$\boldsymbol{\mu} \in \mathcal{M} \Leftrightarrow \begin{cases} \boldsymbol{\mu} \text{ is the null measure on } E \\ \text{or} \\ \exists \mathbf{x}_1, \ldots, \mathbf{x}_N \in E \text{ pairwise distinct, and } \mu_1, \ldots, \mu_N \in (\mathbb{R} - \{0\}),\ \boldsymbol{\mu} = \sum_{k=1}^{N} \mu_k \delta_{\mathbf{x}_k} \end{cases}$$

  $\mathcal{M}$ is obviously a real vector space a base of which is $\{\delta_{\mathbf{x}} : \mathbf{x} \in E\}$.

- $\boldsymbol{\mu}(f) = \sum_{k=1}^{N} \mu_k f(\mathbf{x}_k)$ the integral of any $f \in \mathbb{R}^E$ against any $\boldsymbol{\mu} = \sum_{k=1}^{N} \mu_k \delta_{\mathbf{x}_k} \in \mathcal{M}$
- $\mathcal{M}_{\mathbb{P}}$ the subspace of measures lying in $\mathcal{M}$ vanishing on $\mathbb{P}$:

$$\boldsymbol{\mu} \in \mathcal{M}_{\mathbb{P}} \Leftrightarrow \boldsymbol{\mu}(p) = 0,\ \forall p \in \mathbb{P}$$

- If we are given $\mathbf{X} \subset E$,
  - $\mathcal{M}(\mathbf{X}) = \{\boldsymbol{\lambda} = \sum_{l=1}^{L} \lambda_l \delta_{\mathbf{x}_l} : (\lambda_1, \mathbf{x}_1), \ldots, (\lambda_L, \mathbf{x}_L) \in \mathbb{R} \times \mathbf{X}\}$
  - $\mathcal{M}_{\mathbb{P}}(\mathbf{X}) = \mathcal{M}(\mathbf{X}) \cap \mathcal{M}_{\mathbb{P}}$

2.2 $\mathbb{P}$-unisolvent set

Definition 2.2 $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset E$ *is said to be $\mathbb{P}$-unisolvent if the linear application*

$$L^{\mathbf{X}} : p \in \mathbb{P} \mapsto (p(\mathbf{x}_1), \ldots, p(\mathbf{x}_N)) \in \mathbb{R}^N$$

is injective, or equivalently, if the only $p \in \mathbb{P}$ which vanishes on every $\mathbf{x} \in \mathbf{X}$ is $0 \in \mathbb{P}$.

In this paper, we will always assume that $\mathbb{P}$ is such that $\mathbb{P}$-unisolvent sets exist.

Recalling that $\dim(\mathbb{P}) = n$, elementary arguments lead to:

Lemma 2.1 *A $\mathbb{P}$-unisolvent set is minimal if and only if it contains exactly n elements.*

Now, let

$$\boldsymbol{\Xi} = \{\boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_n\}$$

be a minimal $\mathbb{P}$-unisolvent set.
Since $L^{\boldsymbol{\Xi}}$ is a bijection, the relations

$$\left\{ \begin{array}{lcll} h_k^{\boldsymbol{\Xi}}(\boldsymbol{\xi}_j) & = & 1 & \text{if } j = k \\ h_k^{\boldsymbol{\Xi}}(\boldsymbol{\xi}_j) & = & 0 & \text{otherwise} \end{array} \right. , \ k = 1, \ldots, n$$

which are equivalent to

$$L_{\mathbb{P}}^{\boldsymbol{\Xi}}(h_k^{\boldsymbol{\Xi}}) = \mathbf{e}_k, k = 1, \ldots, n$$

where $\mathbf{e}_k$ is the kth vector of the $\mathbb{R}^n$ canonical basis, define a $\mathbb{P}$ basis $(h_1^{\boldsymbol{\Xi}}, \ldots, h_n^{\boldsymbol{\Xi}})$.
Let us then define

$$\boldsymbol{\pi}^{\boldsymbol{\Xi}} : f \in \mathbb{R}^E \mapsto \sum_{k=1}^{n} f(\boldsymbol{\xi}_k) h_k^{\boldsymbol{\Xi}} \in \mathbb{P}.$$

This immediately follows:

Proposition 2.1 *$\boldsymbol{\pi}^{\boldsymbol{\Xi}}$ is a projector on $\mathbb{P}$, and, for all $f \in \mathbb{R}^E$, $\boldsymbol{\pi}^{\boldsymbol{\Xi}}(f)$ interpolates f on $\boldsymbol{\Xi}$.*

For any element $\mathbf{x}$ of E, let us introduce

$$\delta_{\mathbf{x}}^{\boldsymbol{\Xi}} = \delta_{\mathbf{x}} - \sum_{i=1}^{n} h_i^{\boldsymbol{\Xi}}(\mathbf{x}) \delta_{\boldsymbol{\xi}_i}.$$

Obviously:

- $\delta_{\boldsymbol{\xi}_k}^{\boldsymbol{\Xi}} = 0, \ k = 1, \ldots, n$
- $\delta_{\mathbf{x}}^{\boldsymbol{\Xi}} \in \mathcal{M}_{\mathbb{P}}$, since

$$\delta_{\mathbf{x}}^{\boldsymbol{\Xi}}(h_k^{\boldsymbol{\Xi}}) = \delta_{\mathbf{x}}(h_k^{\boldsymbol{\Xi}}) - \sum_{i=1}^{n} h_i^{\boldsymbol{\Xi}}(\mathbf{x}) \delta_{\boldsymbol{\xi}_i}(h_k^{\boldsymbol{\Xi}}) = h_k^{\boldsymbol{\Xi}}(\mathbf{x}) - \sum_{i=1}^{n} h_i^{\boldsymbol{\Xi}}(\mathbf{x}) h_k^{\boldsymbol{\Xi}}(\boldsymbol{\xi}_i) = h_k^{\boldsymbol{\Xi}}(\mathbf{x}) - h_k^{\boldsymbol{\Xi}}(\mathbf{x}) = 0\,.$$

We then establish this technical proposition that will be useful in the sequel.

Proposition 2.2 *Let $\boldsymbol{\Xi} = \{\boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_n\}$ be any minimal $\mathbb{P}$-unisolvent set. Every $\boldsymbol{\lambda} = \sum_{l=1}^{L} \lambda_l \delta_{\mathbf{x}_l} \in \mathcal{M}$ has the alternative form:*

$$\boldsymbol{\lambda} = \sum_{l=1}^{L} \lambda_l \delta_{\mathbf{x}_l}^{\boldsymbol{\Xi}} + \sum_{k=1}^{n} \boldsymbol{\lambda}(h_k^{\boldsymbol{\Xi}}) \delta_{\boldsymbol{\xi}_k} \tag{2.1}$$

As a consequence,

- $\mathcal{M}_{\mathbb{P}}(\boldsymbol{\Xi}) = \{0\}$
- *for any $\mathbf{X} \subset E$, such that $\boldsymbol{\Xi} \subset \mathbf{X}$, $\{\delta_{\mathbf{x}}^{\boldsymbol{\Xi}} : \mathbf{x} \in \mathbf{X} - \boldsymbol{\Xi}\}$ is a $\mathcal{M}_{\mathbb{P}}(\mathbf{X})$-basis.*

Proof
We readily have:

$$\sum_{l=1}^{L}\lambda_l\delta^{\boldsymbol{\Xi}}_{\mathbf{x}_l}=\sum_{l=1}^{L}\lambda_l(\delta_{\mathbf{x}_l}-\sum_{k=1}^{n}h^{\boldsymbol{\Xi}}_k(\mathbf{x}_l)\delta_{\boldsymbol{\xi}_k})=\sum_{l=1}^{L}\lambda_l\delta_{\mathbf{x}_l}-\sum_{l=1}^{L}\sum_{k=1}^{n}\lambda_l h^{\boldsymbol{\Xi}}_k(\mathbf{x}_l)\delta_{\boldsymbol{\xi}_k}=\boldsymbol{\lambda}-\sum_{k=1}^{n}\left[\sum_{l=1}^{L}\lambda_l h^{\boldsymbol{\Xi}}_k(\mathbf{x}_l)\right]\delta_{\boldsymbol{\xi}_k}$$
$$=\boldsymbol{\lambda}-\sum_{k=1}^{n}\boldsymbol{\lambda}(h^{\boldsymbol{\Xi}}_k)\delta_{\boldsymbol{\xi}_k}$$

hence (2.1). $\mathcal{M}_{\mathbb{P}}(\boldsymbol{\Xi})=\{0\}$ follows immediately.
Let $\mathbf{X}$ be a subset of E which contains $\boldsymbol{\Xi}$.
Any $\boldsymbol{\lambda}=\sum_{i=1}^{N}\lambda_i\delta_{\mathbf{x}_i}\in\mathcal{M}_{\mathbb{P}}(\mathbf{X})$ can be written, using (2.1): $\boldsymbol{\lambda}=\sum_{l=1}^{L}\lambda_l\delta^{\boldsymbol{\Xi}}_{\mathbf{x}_l}$.
Thus, since $\delta^{\boldsymbol{\Xi}}_{\mathbf{x}}\in\mathcal{M}_{\mathbb{P}}(\mathbf{X}),\mathbf{x}\in\mathbf{X}$, $\{\delta^{\boldsymbol{\Xi}}_{\mathbf{x}}:\mathbf{x}\in\mathbf{X}-\boldsymbol{\Xi}\}$ spans $\mathcal{M}_{\mathbb{P}}(\mathbf{X})$.
Moreover, $\{\delta^{\boldsymbol{\Xi}}_{\mathbf{x}}:\ \mathbf{x}\in(\mathbf{X}-\boldsymbol{\Xi})\}$ are linearly independent.
Indeed, let $\mathbf{x}_1,\ldots,\mathbf{x}_N$ be N pairwise distinct elements of $\mathbf{X}-\boldsymbol{\Xi}$. For $(\alpha_1,\ldots,\alpha_N)\in\mathbb{R}^N$ we have from (2.1):

$$\sum_{k=1}^{N}\alpha_k\delta^{\boldsymbol{\Xi}}_{\mathbf{x}_k}=\sum_{k=1}^{N}\alpha_k\delta_{\mathbf{x}_k}-\sum_{i=1}^{n}\left[\sum_{k=1}^{N}\alpha_k h^{\boldsymbol{\Xi}}_i(\mathbf{x}_k)\right]\delta_{\boldsymbol{\xi}_i}\,.$$

But $\mathbf{x}_1,\ldots,\mathbf{x}_N,\boldsymbol{\xi}_1,\ldots,\boldsymbol{\xi}_n$ are distinct, thus $\delta_{\mathbf{x}_1},\ldots,\delta_{\mathbf{x}_N},\delta_{\boldsymbol{\xi}_1},\ldots,\delta_{\boldsymbol{\xi}_n}$ are linearly independent and

$$\sum_{k=1}^{N}\alpha_k\delta^{\boldsymbol{\Xi}}_{\mathbf{x}_k}=0\Rightarrow\sum_{k=1}^{N}\alpha_k\delta_{\mathbf{x}_k}-\sum_{i=1}^{n}\left[\sum_{k=1}^{N}\alpha_k h^{\boldsymbol{\Xi}}_i(\mathbf{x}_k)\right]\delta_{\boldsymbol{\xi}_i}=0\Rightarrow\alpha_k=0,k=1,\ldots,N\,.$$

□
Let us now define:

$$\Phi^{\boldsymbol{\Xi}}:\boldsymbol{\mu}\in\mathcal{M}\mapsto\boldsymbol{\mu}-\sum_{k=1}^{n}\boldsymbol{\mu}(h^{\boldsymbol{\Xi}}_k)\delta_{\boldsymbol{\xi}_k}\in\mathcal{M}.$$

The following facts are obvious:

- $\Phi^{\boldsymbol{\Xi}}(\sum_{i=1}^{N}\lambda_i\delta_{\mathbf{x}_i})=\sum_{i=1}^{N}\lambda_i\delta^{\boldsymbol{\Xi}}_{\mathbf{x}_i}$
- the relation (2.1) can be rephrased as

$$\boldsymbol{\lambda}=\Phi^{\boldsymbol{\Xi}}(\boldsymbol{\lambda})+\sum_{k=1}^{n}\boldsymbol{\lambda}(h^{\boldsymbol{\Xi}}_k)\delta_{\boldsymbol{\xi}_k}$$

- $\Phi^{\boldsymbol{\Xi}}$ is a projection on $\mathcal{M}_{\mathbb{P}}$.

3 Bilinear forms induced by K

Let $\boldsymbol{\mu}=\sum_{m=1}^{M}\mu_m\delta_{\mathbf{x}_m}$ and $\boldsymbol{\lambda}=\sum_{l=1}^{L}\lambda_l\delta_{\mathbf{z}_l}$ be two measures taken in $\mathcal{M}$.
The formula

$$<\boldsymbol{\mu},\boldsymbol{\lambda}>_{\mathcal{M},K}=\sum_{m=1}^{M}\sum_{l=1}^{L}\mu_m\lambda_l K(\mathbf{x}_m,\mathbf{z}_l)$$

defines a symmetric bilinear form $<,>_{\mathcal{M},K}$ on $\mathcal{M}$.
$\mathbb{P}$-conditional positiveness of K means that the restriction of $<,>_{\mathcal{M},K}$ to $\mathcal{M}_{\mathbb{P}}$ is positive.

Kernel K also induces a natural linear application

$$F_K : \boldsymbol{\mu} = \sum_{m=1}^{M} \mu_m \delta_{\mathbf{x}_m} \in \mathcal{M} \mapsto \sum_{m=1}^{M} \mu_m K_{\mathbf{x}_m} \in \mathbb{R}^E.$$

For any $\mathbf{X} \subset E$, let us then set

$$\mathcal{F}_K(\mathbf{X}) = F_K(\mathcal{M}(\mathbf{X}))$$

and

$$\mathcal{F}_{K,\mathbb{P}}(\mathbf{X}) = F_K(\mathcal{M}_{\mathbb{P}}(\mathbf{X}))$$

which will be merely denoted $\mathcal{F}_K$ and $\mathcal{F}_{K,\mathbb{P}}$ when $\mathbf{X} = E$.

Using F_K, we can carry the bilinear structure from $\mathcal{M}$ to $\mathcal{F}_K$:

Proposition 3.1 *Let f, g be functions in $\mathcal{F}_K$ and $\boldsymbol{\lambda}, \boldsymbol{\mu} \in \mathcal{M}$ such that $f = F_K(\boldsymbol{\lambda})$ and $g = F_K(\boldsymbol{\mu})$.*
The formula

$$< f, g >_{\mathcal{F}_K} = < \boldsymbol{\lambda}, \boldsymbol{\mu} >_{\mathcal{M},K}$$

only depends on f and g, and not on the particular choice of $\boldsymbol{\lambda}, \boldsymbol{\mu}$.
Thus it defines a symmetric bilinear form on $\mathcal{F}_K$ whose restriction to $\mathcal{F}_{K,\mathbb{P}}$ is positive.
This reproducing formula is satisfied for any $g \in \mathcal{F}_K$ and $\mathbf{x} \in E$:

$$< K_{\mathbf{x}}, g >_{\mathcal{F}_K} = g(\mathbf{x}). \tag{3.1}$$

Proof
Let us start with

Lemma 3.1 *For every $\boldsymbol{\lambda}, \boldsymbol{\mu} \in \mathcal{M}$,*

$$< \boldsymbol{\lambda}, \boldsymbol{\mu} >_{\mathcal{M},K} = \boldsymbol{\lambda}(F_K(\boldsymbol{\mu})). \tag{3.2}$$

Proof
Let $\boldsymbol{\lambda} = \sum_{l=1}^{L} \lambda_l \delta_{\mathbf{x}_l}$ and $\boldsymbol{\mu} = \sum_{m=1}^{M} \mu_m \delta_{\mathbf{z}_m}$ be the expressions of $\boldsymbol{\lambda}$ and $\boldsymbol{\mu}$ in the $\mathcal{M}$ basis $\{\delta_{\mathbf{x}} : \mathbf{x} \in E\}$.
We readily have:

$$\boldsymbol{\lambda}(F_K(\boldsymbol{\mu})) = \sum_{l=1}^{L} \lambda_l \delta_{\mathbf{x}_l} (\sum_{m=1}^{M} \mu_m K_{\mathbf{z}_m}) = \sum_{l=1}^{L} \sum_{m=1}^{M} \lambda_l \mu_m K(\mathbf{x}_l, \mathbf{z}_m) = < \boldsymbol{\lambda}, \boldsymbol{\mu} >_{\mathcal{M},K} .$$

$\square$
From (3.2) we have

$$\begin{aligned} < \boldsymbol{\lambda}, \boldsymbol{\mu} >_{\mathcal{M},K} &= \boldsymbol{\lambda}(F_K(\boldsymbol{\mu})) = \boldsymbol{\lambda}(g) \\ &= \boldsymbol{\mu}(F_K(\boldsymbol{\lambda})) = \boldsymbol{\mu}(f) \end{aligned}$$

and $< f, g >_{\mathcal{F}_K}$ only depends on f and g.

Now, since the restriction of $<,>_{\mathcal{M},K}$ to $\mathcal{M}_{\mathbb{P}}$ is positive, taking $f = F_K(\boldsymbol{\lambda}) \in \mathcal{F}_{K,\mathbb{P}}$ with $\boldsymbol{\lambda} \in \mathcal{M}_{\mathbb{P}}$ leads to:

$$0 \leq < \boldsymbol{\lambda}, \boldsymbol{\lambda} >_{\mathcal{M},K} = < f, f >_{\mathcal{F}_K}$$

and the restriction of $<,>_{\mathcal{F}_K}$ to $\mathcal{F}_{K,\mathbb{P}}$ is positive.
Applied to $g = F_K(\boldsymbol{\mu})$ and $f = K_{\mathbf{x}} = F_K(\delta_{\mathbf{x}})$, (3.2) leads to the reproducing formula:

$$< K_{\mathbf{x}}, g >_{\mathcal{F}_K} = < \delta_{\mathbf{x}}, \boldsymbol{\mu} >_{\mathcal{M},K} = \delta_{\mathbf{x}}(F_K(\boldsymbol{\mu})) = g(\mathbf{x})\,.$$

□

From K and a minimal $\mathbb{P}$-unisolvent set $\boldsymbol{\Xi}$, we introduce the new kernel $K^{\boldsymbol{\Xi}}$:

$$K^{\boldsymbol{\Xi}} : (\mathbf{x}, \mathbf{x}') \in E^2 \mapsto < \delta^{\boldsymbol{\Xi}}_{\mathbf{x}}, \delta^{\boldsymbol{\Xi}}_{\mathbf{x}'} >_{\mathcal{M},K}\ .$$

This simple calculation:

$$\sum_{1 \leq i,j \leq N} \lambda_i \lambda_j K^{\boldsymbol{\Xi}}(\mathbf{x}, \mathbf{x}') = \sum_{1 \leq i,j \leq N} \lambda_i \lambda_j < \delta^{\boldsymbol{\Xi}}_{\mathbf{x}_i}, \delta^{\boldsymbol{\Xi}}_{\mathbf{x}_j} >_{\mathcal{M},K} = < \sum_{i=1}^{N} \lambda_i \delta^{\boldsymbol{\Xi}}_{\mathbf{x}_i}, \sum_{i=1}^{N} \lambda_i \delta^{\boldsymbol{\Xi}}_{\mathbf{x}_i} >_{\mathcal{M},K} \geq 0$$

leads to

Proposition 3.2 $K^{\boldsymbol{\Xi}}$ *is a (unconditionally) positive kernel.*

We now sum up the main relations between bilinear structures induced by a conditionally positive kernel we met up to this point. This summary consists in the following commutative diagram:

$$\begin{tikzcd}
(\mathcal{M}_{\mathbb{P}}(\mathbf{X}), <,>_{\mathcal{M},K}) \arrow[d, "F_K"'] \arrow[dr, "F_K^{\boldsymbol{\Xi}}"] & \big(\mathcal{M}(\mathbf{X}), <,>_{\mathcal{M},K^{\boldsymbol{\Xi}}}\big) \arrow[l, "\Phi^{\boldsymbol{\Xi}}"'] \arrow[d, "F_{K^{\boldsymbol{\Xi}}}"] \\
(\mathcal{F}_{K,\mathbb{P}}(\mathbf{X}), <,>_{\mathcal{F}_K}) \arrow[r, "\mathrm{Id} - \boldsymbol{\pi}^{\boldsymbol{\Xi}}"] & \big(\mathcal{F}_{K^{\boldsymbol{\Xi}}}(\mathbf{X}), <,>_{\mathcal{F}_{K^{\boldsymbol{\Xi}}}}\big)
\end{tikzcd} \tag{3.3}$$

where

- $\mathbf{X}$ is any subset of E
- $\boldsymbol{\Xi} \subset \mathbf{X}$ is a minimal $\mathbb{P}$-unisolvent set
- $F_{K^{\boldsymbol{\Xi}}}$ and $\mathcal{F}_{K^{\boldsymbol{\Xi}}}$ are the analogs of F_K and $\mathcal{F}_K$ whith $K^{\boldsymbol{\Xi}}$ in place of K.

- $F_K^{\Xi} : \mathcal{M} \mapsto \mathbb{R}^E$ is specified by

$$F_K^{\Xi}(\boldsymbol{\lambda}) : \mathbf{x} \mapsto < \boldsymbol{\lambda}, \delta_{\mathbf{x}}^{\Xi} >_{\mathcal{M},K} .$$

The diagram (3.3) must be read with the following conventions:

- Any arrow between two bilinear structures is a morphism for them.
- Any two oriented paths from one structure to another lead to the same composite mapping: e.g. $F_{K^{\Xi}} = F_K^{\Xi} \circ \Phi^{\Xi}$.

The "mapping" part of that diagram is the immediate consequence of the

Proposition 3.3 *For all $\boldsymbol{\lambda} \in \mathcal{M}$,*

$$F_K(\boldsymbol{\lambda}) = \boldsymbol{\pi}^{\Xi}(F_K(\boldsymbol{\lambda})) + F_K^{\Xi}(\boldsymbol{\lambda}), \tag{R_1}$$

$$F_{K^{\Xi}}(\boldsymbol{\lambda}) = F_K^{\Xi}(\Phi^{\Xi}(\boldsymbol{\lambda})). \tag{R_2}$$

Proof
(R_1) follows from this:

$$\begin{aligned}
F_K^{\Xi}(\boldsymbol{\lambda})(\mathbf{x}) &=< \boldsymbol{\lambda}, \delta_{\mathbf{x}}^{\Xi} >_{\mathcal{M},K} \\
&=< \boldsymbol{\lambda}, \delta_{\mathbf{x}} - \sum_{i=1}^{n} h_i^{\Xi}(\mathbf{x})\delta_{\boldsymbol{\xi}_i} >_{\mathcal{M},K} \\
&=< \boldsymbol{\lambda}, \delta_{\mathbf{x}} >_{\mathcal{M},K} - \sum_{i=1}^{n} h_i^{\Xi}(\mathbf{x}) < \boldsymbol{\lambda}, \delta_{\boldsymbol{\xi}_i} >_{\mathcal{M},K} \\
&= F_K(\boldsymbol{\lambda})(\mathbf{x}) - \sum_{i=1}^{n} h_i^{\Xi}(\mathbf{x}) F_K(\boldsymbol{\lambda})(\boldsymbol{\xi}_i) \\
&= F_K(\boldsymbol{\lambda})(\mathbf{x}) - \boldsymbol{\pi}^{\Xi}(F_K(\boldsymbol{\lambda}))(\mathbf{x}).
\end{aligned}$$

(R_2) comes from: if $\boldsymbol{\lambda} = \sum_{l=1}^{L} \lambda_l \delta_{\mathbf{x}_l}$

$$\begin{aligned}
F_{K^{\Xi}}(\boldsymbol{\lambda})(\mathbf{x}) &=< \boldsymbol{\lambda}, \delta_{\mathbf{x}} >_{\mathcal{M},K^{\Xi}} = \sum_{l=1}^{L} \lambda_l K^{\Xi}(\mathbf{x}_l, \mathbf{x}) = \sum_{l=1}^{L} \lambda_l < \delta_{\mathbf{x}_l}^{\Xi}, \delta_{\mathbf{x}}^{\Xi} >_{\mathcal{M},K} =< \sum_{l=1}^{L} \lambda_l \delta_{\mathbf{x}_l}^{\Xi}, \delta_{\mathbf{x}}^{\Xi} >_{\mathcal{M},K} \\
&= F_K^{\Xi}(\sum_{l=1}^{L} \lambda_l \delta_{\mathbf{x}_l}^{\Xi})(\mathbf{x}) = F_K^{\Xi}(\Phi^{\Xi}(\boldsymbol{\lambda}))(\mathbf{x}).
\end{aligned}$$

$\square$
The morphism part of (3.3) is easily verified from:

Proposition 3.4 *1. Φ^{Ξ} is a morphism between $(\mathcal{M}(\mathbf{X}), <,>_{\mathcal{M},K^{\Xi}})$ and $(\mathcal{M}_{\mathbb{P}}(\mathbf{X}), <,>_{\mathcal{M},K})$.*

2. $\mathrm{Id} - \boldsymbol{\pi}^{\Xi}$ is a morphism between $(\mathcal{F}_{K,\mathbb{P}}(\mathbf{X}), <,>_{\mathcal{F}_K})$ and $(\mathcal{F}_{K^{\Xi}}(\mathcal{M}(\mathbf{X})), <,>_{\mathcal{F}_{K^{\Xi}}})$.

Proof

1. $< \Phi^{\Xi}(\delta_{\mathbf{x}}), \Phi^{\Xi}(\delta_{\mathbf{x}'}) >_{\mathcal{M},K} = < \delta^{\Xi}_{\mathbf{x}}, \delta^{\Xi}_{\mathbf{x}'} >_{\mathcal{M},K} = K^{\Xi}(\mathbf{x}, \mathbf{x}') = < \delta_{\mathbf{x}}, \delta_{\mathbf{x}'} >_{\mathcal{M},K^{\Xi}}$ leads immediately to
$$< \Phi^{\Xi}(\boldsymbol{\lambda}), \Phi^{\Xi}(\boldsymbol{\mu}) >_{\mathcal{M},K} = < \boldsymbol{\lambda}, \boldsymbol{\mu} >_{\mathcal{M},K^{\Xi}} \tag{3.4}$$
for any $\boldsymbol{\lambda}, \boldsymbol{\mu} \in \mathcal{M}$.

2. Let f and g be two functions in $\mathcal{F}_{K,\mathbb{P}}(\mathbf{X})$: there exists $\boldsymbol{\lambda}, \boldsymbol{\mu} \in \mathcal{M}_{\mathbb{P}}(\mathbf{X})$ such that $f = F_K(\boldsymbol{\lambda})$ and $g = F_K(\boldsymbol{\mu})$.
Recalling that $\boldsymbol{\lambda}, \boldsymbol{\mu} \in \mathcal{M}_{\mathbb{P}}(\mathbf{X}) \Rightarrow \Phi^{\Xi}(\boldsymbol{\lambda}) = \boldsymbol{\lambda},\ \Phi^{\Xi}(\boldsymbol{\mu}) = \boldsymbol{\mu}$, we actually have
$$f = F_K(\Phi^{\Xi}(\boldsymbol{\lambda})) \text{ and } g = F_K(\Phi^{\Xi}(\boldsymbol{\mu}))\,.$$
From Proposition 3.3 it follows
$$f - \boldsymbol{\pi}^{\Xi}(f) = F_{K^{\Xi}}(\Phi^{\Xi}(\boldsymbol{\lambda})) = F_{K^{\Xi}}(\boldsymbol{\lambda})$$
and
$$g - \boldsymbol{\pi}^{\Xi}(g) = F_{K^{\Xi}}(\Phi^{\Xi}(\boldsymbol{\mu})) = F_{K^{\Xi}}(\boldsymbol{\mu})$$
leading to:
$$< f - \boldsymbol{\pi}^{\Xi}(f), g - \boldsymbol{\pi}^{\Xi}(g) >_{\mathcal{F}_{K^{\Xi}}} = < F_{K^{\Xi}}(\boldsymbol{\lambda}), F_{K^{\Xi}}(\boldsymbol{\mu}) >_{\mathcal{F}_{K^{\Xi}}} = < \boldsymbol{\lambda}, \boldsymbol{\mu} >_{\mathcal{M},K^{\Xi}} \ .$$
But F_K definition directly gives:
$$< f, g >_{\mathcal{F}_K} = < F_K(\boldsymbol{\lambda}), F_K(\boldsymbol{\mu}) >_{\mathcal{F}_K} = < \boldsymbol{\lambda}, \boldsymbol{\mu} >_{\mathcal{M},K} = < \Phi^{\Xi}(\boldsymbol{\lambda}), \Phi^{\Xi}(\boldsymbol{\mu}) >_{\mathcal{M},K}$$
then, with (3.4):
$$< f, g >_{\mathcal{F}_K} = < \boldsymbol{\lambda}, \boldsymbol{\mu} >_{\mathcal{M},K^{\Xi}} \ .$$
Hence
$$< f, g >_{\mathcal{F}_K} = < f - \boldsymbol{\pi}^{\Xi}(f), g - \boldsymbol{\pi}^{\Xi}(g) >_{\mathcal{F}_{K^{\Xi}}} \ .$$

□

Remark 1 *These consequences of diagram (3.3) will be often used in the sequel:*
$$\forall f \in \mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X}), f - \boldsymbol{\pi}^{\Xi}(f) \in \mathcal{F}_{K^{\Xi}}(\mathbf{X}), \tag{3.5}$$
$$\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X}) = \mathbb{P} + \mathcal{F}_{K^{\Xi}}(\mathbf{X}). \tag{3.6}$$
Indeed, if $f \in \mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X})$, we can write $f = p + g$ with $p \in \mathbb{P}$ and $g \in \mathcal{F}_{K,\mathbb{P}}(\mathbf{X})$. So, $f - \boldsymbol{\pi}^{\Xi}(f) = p + g - p - \boldsymbol{\pi}^{\Xi}(g) = g - \boldsymbol{\pi}^{\Xi}(g)$, and diagram (3.3) gives
$$g - \boldsymbol{\pi}^{\Xi}(g) \in \mathcal{F}_{K^{\Xi}}(\mathbf{X})$$
hence (3.5).
Now (3.5) implies
$$\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X}) \subset \mathbb{P} + \mathcal{F}_{K^{\Xi}}(\mathbf{X})\,.$$
Moreover, since $F_{K^{\Xi}}$ is an onto mapping from $\mathcal{M}(\mathbf{X})$ on $\mathcal{F}_{K^{\Xi}}(\mathbf{X})$, so is the mapping $\mathrm{Id} - \boldsymbol{\pi}^{\Xi}$ between $\mathcal{F}_{K,\mathbb{P}}(\mathbf{X})$, hence
$$\mathbb{P} + \mathcal{F}_{K^{\Xi}}(\mathbf{X}) \subset \mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X})\,.$$
Thus (3.6).

4 $\mathbb{P}$-reproducing kernel semi-Hilbert space

4.1 $\mathbb{P}$-conditionally positive definite kernel

We know from Proposition 3.1 that, K being $\mathbb{P}$-conditionally positive, $<,>_{\mathcal{F}_K}$ is a positive symmetric bilinear form on $\mathcal{F}_{K,\mathbb{P}}$.
Here is a characterization of couples $(K, \mathbb{P})$ which leads to the positive definiteness of $<,>_{\mathcal{F}_K}$ on $\mathcal{F}_{K,\mathbb{P}}$.

Proposition 4.1 *For any $f \in \mathcal{F}_{K,\mathbb{P}}$,*

$$< f, f >_{\mathcal{F}_K} = 0 \Leftrightarrow f \in \mathbb{P}\,.$$

Hence $<,>_{\mathcal{F}_K}$ is positive definite on $\mathcal{F}_{K,\mathbb{P}}$ if and only if $\mathbb{P} \cap \mathcal{F}_{K,\mathbb{P}} = \{0\}$.

Proof
Let us first set this well known property:

Lemma 4.1 *If R is a positive kernel, then $<,>_{\mathcal{F}_R}$ is positive definite.*

Proof
Let $g \in \mathcal{F}_R$.
Reproducing property (3.1) and Cauchy-Schwarz inequality leads to:

$$|g(\mathbf{x})| = |< R_{\mathbf{x}}, g >_{\mathcal{F}_R}| = \sqrt{< g, g >_{\mathcal{F}_R}}\sqrt{< R_{\mathbf{x}}, R_{\mathbf{x}} >_{\mathcal{F}_R}}\,.$$

Hence, $< g, g >_{\mathcal{F}_R} = 0 \Rightarrow \forall \mathbf{x} \in E, g(\mathbf{x}) = 0 \Rightarrow g = 0$.
□
Now, let $f \in \mathcal{F}_{K,\mathbb{P}}$ and $\boldsymbol{\lambda} \in \mathcal{M}_{\mathbb{P}}$ be such that $f = F_K(\boldsymbol{\lambda})$.
From (3.2), we get:

$$< f, f >_{\mathcal{F}_{K,\mathbb{P}}} = < \boldsymbol{\lambda}, \boldsymbol{\lambda} >_{\mathcal{M},K} = \boldsymbol{\lambda}(F_K(\boldsymbol{\lambda})). \tag{4.1}$$

Since $\boldsymbol{\lambda} \in \mathcal{M}_{\mathbb{P}}$, it follows that $\Phi^{\boldsymbol{\Xi}}(\boldsymbol{\lambda}) = \boldsymbol{\lambda}$ and, then, diagram (3.3) implies

$$F_K(\boldsymbol{\lambda}) = \boldsymbol{\pi}^{\boldsymbol{\Xi}}(F_K(\boldsymbol{\lambda})) + F_{K^{\boldsymbol{\Xi}}}(\boldsymbol{\lambda}). \tag{4.2}$$

Applying $\boldsymbol{\lambda}$ to both terms of (4.2), leads to

$$\boldsymbol{\lambda}(F_K(\boldsymbol{\lambda})) = \boldsymbol{\lambda}(F_{K^{\boldsymbol{\Xi}}}(\boldsymbol{\lambda}))$$

since $\boldsymbol{\lambda} \in \mathcal{M}_{\mathbb{P}}$ implies that $\boldsymbol{\lambda}(\boldsymbol{\pi}^{\boldsymbol{\Xi}}(F_K(\boldsymbol{\lambda}))) = 0$.
Equality (4.1) then becomes

$$< f, f >_{\mathcal{F}_{K,\mathbb{P}}} = \boldsymbol{\lambda}(F_{K^{\boldsymbol{\Xi}}}(\boldsymbol{\lambda})) = < F_{K^{\boldsymbol{\Xi}}}(\boldsymbol{\lambda}), F_{K^{\boldsymbol{\Xi}}}(\boldsymbol{\lambda}) >_{\mathcal{F}_{K^{\boldsymbol{\Xi}}}}\,.$$

Hence

$$< f, f >_{\mathcal{F}_{K,\mathbb{P}}} = 0 \Leftrightarrow < F_{K^{\boldsymbol{\Xi}}}(\boldsymbol{\lambda}), F_{K^{\boldsymbol{\Xi}}}(\boldsymbol{\lambda}) >_{\mathcal{F}_{K^{\boldsymbol{\Xi}}}} = 0\,.$$

which, with Lemma 4.1 applied to $K^{\boldsymbol{\Xi}}$, leads to

$$< f, f >_{\mathcal{F}_{K,\mathbb{P}}} = 0 \Leftrightarrow F_{K^{\boldsymbol{\Xi}}}(\boldsymbol{\lambda}) = 0$$

Eventually, from (4.2)

$$< f, f >_{\mathcal{F}_{K,\mathbb{P}}} = 0 \Leftrightarrow f = \boldsymbol{\pi}^{\boldsymbol{\Xi}}(f) \Leftrightarrow f \in \mathbb{P}$$

□
We are naturally led to the following definition:

Definition 4.1 ($\mathbb{P}$-conditionally positive definite kernel) *A $\mathbb{P}$-conditionally positive kernel K is said $\mathbb{P}$-conditionally positive* **definite** *if*

$$\mathbb{P} \cap \mathcal{F}_{K,\mathbb{P}} = \{0\}.$$

In other words: K is $\mathbb{P}$-conditionally positive definite if and only if $<,>_{\mathcal{F}_K}$ is a positive definite symmetric bilinear form on $\mathcal{F}_{K,\mathbb{P}}$.

Here are three particular cases where $\mathbb{P} \cap \mathcal{F}_{K,\mathbb{P}} = \{0\}$ and consequently where K is $\mathbb{P}$-conditionally positive definite.

1. $\mathbb{P} = \{0\}$.
   It is the classical case of positive definite kernel. There is no differences between positive kernel and positive definite kernel.

2. More generally, whatever $\mathbb{P}$ is, if K is positive then it is $\mathbb{P}$-conditionally positive definite.
   Indeed, let f be in $\mathbb{P} \cap \mathcal{F}_{K,\mathbb{P}}$. Since $f \in \mathcal{F}_{K,\mathbb{P}}$, there exists $\boldsymbol{\lambda} \in \mathcal{M}_{\mathbb{P}}$ such that $f = F_K(\boldsymbol{\lambda})$. We have, using (3.2)

   $$< f, f >_{\mathcal{F}_K} = < \boldsymbol{\lambda}, \boldsymbol{\lambda} >_{\mathcal{M},K} = \boldsymbol{\lambda}(F_K(\boldsymbol{\lambda})) = \boldsymbol{\lambda}(f) = 0$$

   since $f \in \mathbb{P}$.
   But, K positive implies that $<,>_{\mathcal{F}_K}$ is positive definite (see Lemma 4.1), hence

   $$< f, f >_{\mathcal{F}_K} = 0 \Rightarrow f = 0\,.$$

3. The following condition is the $\mathbb{P}$-conditionally positive definite kernel definition given in [11]: for all $L \in \mathbb{N}$, and every $\mathbf{x}_1, \ldots, \mathbf{x}_L$ **pairwise distinct**

   $$\forall(\lambda_1, \ldots, \lambda_L) \in \mathbb{R}^L \left\{ \begin{array}{c} \sum_{1 \le k,l=L} \lambda_l \lambda_k K(\mathbf{x}_l, \mathbf{x}_k) = 0 \\ \text{et} \\ \sum_{l=1}^{L} \lambda_l p(\mathbf{x}_l) = 0, \forall p \in \mathbb{P} \end{array} \right. \Rightarrow \lambda_l = 0, l = 1, \ldots, L. \tag{4.3}$$

   Indeed, suppose $K, \mathbb{P}$ are satisfying (4.3) and let f be in $\mathbb{P} \cap \mathcal{F}_{K,\mathbb{P}}$.
   On the one hand $f \in \mathcal{F}_{K,\mathbb{P}}$. Hence there exists $\boldsymbol{\mu} \in \mathcal{M}_{\mathbb{P}}$ such that $f = F_K(\boldsymbol{\mu})$.
   On the other hand $f \in \mathbb{P}$, thus $\boldsymbol{\mu}(f) = 0$.
   Combining these two facts we get

   $$\boldsymbol{\mu}(F_K(\boldsymbol{\mu})) = 0. \tag{4.4}$$

   Let us now write $\boldsymbol{\mu} = \sum_{m=1}^{M} \mu_k \delta_{\mathbf{x}_k}$, with $\{\mathbf{x}_1, \ldots, \mathbf{x}_M\}$ pairwise distinct.
   Relation (4.4) becomes:

   $$\sum_{m,l} \mu_l \mu_m K(\mathbf{x}_l, \mathbf{x}_m) = 0\,.$$

   Since $\boldsymbol{\mu} \in \mathcal{M}_{\mathbb{P}}$, it follows from (4.3) that $\mu_k = 0, k = 1, \ldots, M$, then $\boldsymbol{\mu} = 0$ and eventually $f = 0$.

Let us notice that condition (4.3) cannot be satisfied if $\mathcal{F}_{K,\mathbb{P}}$ is a finite-dimensional vector space, and say E infinite.
Indeed, suppose $\mathcal{F}_{K,\mathbb{P}}$ is a finite-dimensional vector space.
Let $\boldsymbol{\Xi} = \{\boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_n\}$ be a minimal $\mathbb{P}$-unisolvent set. There exists $\mathbf{x}_1, \ldots, \mathbf{x}_L \in E - \boldsymbol{\Xi}$ pairwise distinct such that $F_K(\delta^{\boldsymbol{\Xi}}_{\mathbf{x}_1}), \ldots, F_K(\delta^{\boldsymbol{\Xi}}_{\mathbf{x}_L})$, which all are in $\mathcal{F}_{K,\mathbb{P}}$, are linearly dependent:

$$\exists(\lambda_1, \ldots, \lambda_L) \neq 0 \in \mathbb{R}^L \text{such that } \sum_{l=1}^{L} \lambda_l F_K(\delta^{\boldsymbol{\Xi}}_{\mathbf{x}_l}) = 0. \tag{4.5}$$

Hence

$$0 =< F_K(\sum_{l=1}^{L} \lambda_l \delta^{\boldsymbol{\Xi}}_{\mathbf{x}_l}), F_K(\sum_{l=1}^{L} \lambda_l \delta^{\boldsymbol{\Xi}}_{\mathbf{x}_l}) >_{\mathcal{F}_K} \; =< \sum_{l=1}^{L} \lambda_l \delta^{\boldsymbol{\Xi}}_{\mathbf{x}_l}, \sum_{l=1}^{L} \lambda_l \delta^{\boldsymbol{\Xi}}_{\mathbf{x}_l} >_{\mathcal{M},K} . \tag{4.6}$$

Since $\sum_{l=1}^{L} \lambda_l \delta^{\boldsymbol{\Xi}}_{\mathbf{x}_l} = \sum_{l=1}^{L} \lambda_l \delta_{\mathbf{x}_l} - \sum_{k=1}^{n} \left[\sum_{l=1}^{L} \lambda_l h^{\boldsymbol{\Xi}}_k(\mathbf{x}_l) \right] \delta_{\boldsymbol{\xi}_k}$ we can write

$$\sum_{l=1}^{L} \lambda_l \delta^{\boldsymbol{\Xi}}_{\mathbf{x}_l} = \sum_{l=1}^{L+n} \lambda_l \delta_{\mathbf{x}_l}$$

where $\lambda_{L+k} = -\sum_{l=1}^{L} \lambda_l h^{\boldsymbol{\Xi}}_k(\mathbf{x}_l)$ and $\mathbf{x}_{L+k} = \boldsymbol{\xi}_k,\ k = 1, \ldots n$. And (4.6) becomes:

$$0 =< \sum_{l=1}^{L+n} \lambda_l \delta_{\mathbf{x}_l}, \sum_{l=1}^{L+n} \lambda_l \delta_{\mathbf{x}_l} >_{\mathcal{M},K} = \sum_{1 \le i,j \le L+n} \lambda_i \lambda_j K(\mathbf{x}_i, \mathbf{x}_j) \, .$$

If condition (4.3) were satisfied, recalling $\sum_{l=1}^{L+n} \lambda_l \delta_{\mathbf{x}_l} \in \mathcal{M}_{\mathbb{P}}$, this last equality would imply: $\lambda_i = 0, i = 1, \ldots, L+n$, which conflicts with (4.5).

4.2 $\mathbb{P}$-Reproducing Kernel Semi-Hilbert Space

Here is the main result of our study:

Theorem 4.1 *Assume K is a $\mathbb{P}$-conditionally positive definite kernel. There is a unique semi-Hilbert space of real functions defined on E, $\left(\mathcal{H}_{K,\mathbb{P}}, <,>_{\mathcal{H}_{K,\mathbb{P}}}\right)$ such that*

1. *$\left(\mathcal{F}_{K,\mathbb{P}}, <,>_{\mathcal{F}_{K,\mathbb{P}}}\right)$ is a pre-hilbertian subspace of $\left(\mathcal{H}_{K,\mathbb{P}}, <,>_{\mathcal{H}_{K,\mathbb{P}}}\right)$,*
2. *$\mathbb{P} \subset \mathcal{H}_{K,\mathbb{P}}$ is the null space of $<,>_{\mathcal{H}_{K,\mathbb{P}}}$,*
3. *for all $\boldsymbol{\Xi}$, minimal $\mathbb{P}$-unisolvent set, the following reproducing property is satisfied:*

$$\forall f \in \mathcal{H}_{K,\mathbb{P}},\ \mathbf{x} \in E,\ f(\mathbf{x}) = \boldsymbol{\pi}^{\boldsymbol{\Xi}}(f)(\mathbf{x}) + < f, F_K(\delta^{\boldsymbol{\Xi}}_{\mathbf{x}}) >_{\mathcal{H}_{K,\mathbb{P}}} . \tag{4.7}$$

We call $\left(\mathcal{H}_{K,\mathbb{P}}, <,>_{\mathcal{H}_{K,\mathbb{P}}}\right)$ the $\mathbb{P}$-reproducing kernel semi-Hilbert space ($\mathbb{P}$-R.K.S.H.S) associated with $(K, \mathbb{P})$.

By a semi-Hilbert space, we mean:

Definition 4.2 *A vector space $\mathcal{L}$ equipped with a symmetric positive bilinear form $<,>_{\mathcal{L}}$ is semi-hilbertian if, $\mathcal{K}$ being the null subspace*[1] *of $(\mathcal{L},<,>_{\mathcal{L}})$, the quotient space $\mathcal{L}/\mathcal{K}$ endowed with the bilinear form induced by $<,>_{\mathcal{L}}$ is a Hilbert space.*

As a byproduct useful result, we will also get

Proposition 4.2 *Any choice of a minimal $\mathbb{P}$-unisolvent set $\boldsymbol{\Xi}$, leads to the direct sum decomposition:*

$$\mathcal{H}_{K,\mathbb{P}} = \mathbb{P} \bigoplus \mathcal{H}_{K^{\boldsymbol{\Xi}}}$$

with $\boldsymbol{\pi}^{\boldsymbol{\Xi}}$ and $\left(\mathrm{Id}_{\mathcal{H}_{K,\mathbb{P}}} - \boldsymbol{\pi}^{\boldsymbol{\Xi}}\right)$ as associated projectors.
Moreover

$$< f, g >_{\mathcal{H}_{K,\mathbb{P}}} = < f - \boldsymbol{\pi}^{\boldsymbol{\Xi}}(f), g - \boldsymbol{\pi}^{\boldsymbol{\Xi}}(g) >_{\mathcal{H}_{K^{\boldsymbol{\Xi}}}} .$$

Remark 2 *Since $< f, F_K(\delta_{\mathbf{x}}^{\boldsymbol{\Xi}}) >_{\mathcal{H}_{K,\mathbb{P}}} = < f, F_K(\delta_{\mathbf{x}}^{\boldsymbol{\Xi}}) - \boldsymbol{\pi}^{\boldsymbol{\Xi}}(F_K(\delta_{\mathbf{x}}^{\boldsymbol{\Xi}})) >_{\mathcal{H}_{K,\mathbb{P}}} = < f, K_{\mathbf{x}}^{\boldsymbol{\Xi}} >_{\mathcal{H}_{K,\mathbb{P}}}$, the reproducing formula (4.7) can be written:*

$$\forall f \in \mathcal{H}_{K,\mathbb{P}},\ \mathbf{x} \in E,\ f(\mathbf{x}) = \boldsymbol{\pi}^{\boldsymbol{\Xi}}(f)(\mathbf{x}) + < f, K_{\mathbf{x}}^{\boldsymbol{\Xi}} >_{\mathcal{H}_{K,\mathbb{P}}} .$$

4.2.1 Positive definite case

Suppose K is positive and $\mathbb{P} = \{0\}$. Kernel K is also positive definite according to definition 4.1.
Theorem 4.1 reduces to Aronszajn's

Theorem 4.2 *There is a unique Hilbert space of real functions $(\mathcal{H}_K,<,>_{\mathcal{H}_K})$ such that:*

1. *$(\mathcal{F}_K,<,>_{\mathcal{F}_K})$ is a pre-Hilbert subspace of $(\mathcal{H}_K,<,>_{\mathcal{H}_K})$,*
2. *the following reproducing property is satisfied*

$$\forall f \in \mathcal{H}_K,\ \mathbf{x} \in E,\ f(\mathbf{x}) = < f, K_{\mathbf{x}} >_{\mathcal{H}_K} . \tag{4.8}$$

$\mathcal{H}_K$ is the reproducing kernel Hilbert space (R.K.H.S) with reproducing kernel K.

Proof
Existence
$<,>_{\mathcal{F}_K}$ being positive definite on $\mathcal{F}_K$, let $(\mathcal{H},<,>_{\mathcal{H}})$ be the Hilbert completion of $(\mathcal{F}_K,<,>_{\mathcal{F}_K})$.

Lemma 4.2 *The mapping*

$$R : h \in \mathcal{H} \mapsto \{\mathbf{x} \mapsto < h, K_{\mathbf{x}} >_{\mathcal{H}}\} \in \mathbb{R}^E$$

is an injection.

[1] $\mathcal{K} = \{\mathbf{u} \in \mathcal{L} :< \mathbf{u}, \mathbf{v} >_{\mathcal{L}} = 0, \forall \mathbf{v} \in \mathcal{L}\} = \{\mathbf{u} \in \mathcal{L} :< \mathbf{u}, \mathbf{u} >_{\mathcal{L}} = 0\}$

Proof
The set $\{K_{\mathbf{x}} : \mathbf{x} \in E\}$ is total in $\mathcal{H}$, since it spans $\mathcal{F}_K$ which is dense in $\mathcal{H}$.
Hence

$$R(h) = 0 \Leftrightarrow < h, K_{\mathbf{x}} >_{\mathcal{H}} = 0,\ \forall \mathbf{x} \in E \Leftrightarrow h = 0\,.$$

□
Let $\mathcal{H}_K = R(\mathcal{H})$, be equipped with the following inner product:

$$< R(h_1), R(h_2) >_{\mathcal{H}_K} = < h_1, h_2 >_{\mathcal{H}}\ .$$

$(\mathcal{H}_K, <,>_{\mathcal{H}_K})$ is a Hilbert space as isomorphic image of $\mathcal{H}$.
It satisfies the required properties:

1. $R(K_{\mathbf{x}}) = K_{\mathbf{x}}$ as shown by

$$R(K_{\mathbf{z}})(\mathbf{x}) = < K_{\mathbf{z}}, K_{\mathbf{x}} >_{\mathcal{H}} = < K_{\mathbf{z}}, K_{\mathbf{x}} >_{\mathcal{F}_K} = K(\mathbf{z}, \mathbf{x}) = K_{\mathbf{z}}(\mathbf{x})$$

   implies $R(f) = f$ for any $f \in \mathcal{F}_K$.
   Hence $\mathcal{F}_K \subset \mathcal{H}_K$ which leads readily to first property.

2. Let f be any function in $\mathcal{H}_K$, and $h \in \mathcal{H}$ be such that $R(h) = f$. We have:

$$< f, K_{\mathbf{x}} >_{\mathcal{H}_K} = < R(h), R(K_{\mathbf{x}}) >_{\mathcal{H}_K} = < h, K_{\mathbf{x}} >_{\mathcal{H}} = R(h)(\mathbf{x}) = f(\mathbf{x})\,.$$

Unicity
It comes from this fact:

Lemma 4.3 *If $\mathcal{H}$ is an Hilbert space of functions satisfying the specifications of Theorem 4.2, then $\{K_{\mathbf{x}} : \mathbf{x} \in E\}$ is a total set in $\mathcal{H}$.*

Proof
Let $h \in \mathcal{H}$ be such that

$$\forall \mathbf{x} \in E,\ < h, K_{\mathbf{x}} >_{\mathcal{H}} = 0\,.$$

From the reproduction property (4.8) it follows:

$$\forall \mathbf{x} \in E,\ h(\mathbf{x}) = 0$$

hence $h = 0$
□
Now let $\mathcal{H}$ and $\mathcal{H}'$ be two Hilbert spaces of real functions defined on E, satisfying Theorem 4.2 properties.
From Lemma 4.3, they both contain $(\mathcal{F}_K, <,>_{\mathcal{F}_K})$ as dense subspace.
The identity on $\mathcal{F}_K$ can be then extended as an isometry

$$I : \mathcal{H} \mapsto \mathcal{H}'\,.$$

Hence

$$\forall h \in \mathcal{H}, \mathbf{x} \in E,\ < h, K_{\mathbf{x}} >_{\mathcal{H}} = < I(h), K_{\mathbf{x}} >_{\mathcal{H}'}$$

or

$$\forall h \in \mathcal{H}, \mathbf{x} \in E\ h(\mathbf{x}) = I(h)(\mathbf{x})$$

which means $\forall h \in \mathcal{H}, h = I(h)$
□

4.2.2 General case: existence

Let $\mathbf{\Xi}$ be a minimal $\mathbb{P}$-unisolvent set. Theorem 4.2 can be applied to $K^{\mathbf{\Xi}}$. Observe that any function f of its R.K.H.S satisfies:

$$f(\boldsymbol{\xi}) = 0, \ \forall \boldsymbol{\xi} \in \mathbf{\Xi}\,. \tag{4.9}$$

Indeed, (4.9) is true for $f = K_{\mathbf{x}}^{\mathbf{\Xi}}$ since

$$f(\boldsymbol{\xi}) = K_{\mathbf{x}}^{\mathbf{\Xi}}(\boldsymbol{\xi}) = K^{\mathbf{\Xi}}(\mathbf{x}, \boldsymbol{\xi}) =< \delta_{\mathbf{\Xi}}^{\mathbf{x}}, \delta_{\mathbf{\Xi}}^{\boldsymbol{\xi}} >_{\mathcal{M},K}$$

and $\delta_{\mathbf{\Xi}}^{\boldsymbol{\xi}} = 0$.
Hence it is true for any $f \in \mathcal{F}_{K^{\mathbf{\Xi}}}$.
From Lemma 4.3, $\mathcal{F}_{K^{\mathbf{\Xi}}}$ is dense in $\mathcal{H}_{K^{\mathbf{\Xi}}}$. So any $f \in \mathcal{H}_{K^{\mathbf{\Xi}}}$ can be written as limit of a sequence $(f_k)_{k\in\mathbb{N}}$ of functions of $\mathcal{F}_{K^{\mathbf{\Xi}}}$.
Then for any $\boldsymbol{\xi} \in \mathbf{\Xi}$, we have:

$$f(\boldsymbol{\xi}) =< f, K_{\boldsymbol{\xi}}^{\mathbf{\Xi}} >_{\mathcal{H}_{K^{\mathbf{\Xi}}}} = \lim_{k\to\infty} < f_k, K_{\boldsymbol{\xi}}^{\mathbf{\Xi}} >_{\mathcal{H}_{K^{\mathbf{\Xi}}}} = \lim_{k\to\infty} f_k(\boldsymbol{\xi}) = 0.$$

Hence (4.9) follows.
An immediate consequence of (4.9) is:

Proposition 4.3 *The sum $\mathcal{N} = \mathbb{P} + \mathcal{H}_{K^{\mathbf{\Xi}}}$ is direct.*
Moreover, $\boldsymbol{\pi}^{\mathbf{\Xi}}$ and $\mathrm{Id} - \boldsymbol{\pi}^{\mathbf{\Xi}}$ restricted to $\mathcal{N}$ are the associated projections of this direct sum decomposition.

Moreover:

Proposition 4.4 (existence) $\mathcal{N} = \mathbb{P} \oplus \mathcal{H}_{K^{\mathbf{\Xi}}}$ *with the following bilinear form*

$$<,>_{\mathcal{N}} : (p_1 + h_1, p_2 + h_2) \in [\mathbb{P} \oplus \mathcal{H}_{K^{\mathbf{\Xi}}}]^2 \mapsto < h_1, h_2 >_{\mathcal{H}_{K^{\mathbf{\Xi}}}}$$

satisfies the properties required by Theorem 4.1.

Proof
Equipped with the form induced by $<,>_{\mathcal{N}}$, $\mathcal{N}/\mathbb{P}$ is obviously isomorphic to $\left(\mathcal{H}_{K^{\mathbf{\Xi}}}, <,>_{\mathcal{H}_{K^{\mathbf{\Xi}}}}\right)$: $(\mathcal{N}, <,>_{\mathcal{N}})$ is semi-hilbertian and its null space is $\mathbb{P}$.
From (3.6) we know that

$$\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X}) = \mathbb{P} + \mathcal{F}_{K^{\mathbf{\Xi}}}(\mathbf{X})$$

hence $\mathcal{F}_{K,\mathbb{P}}(\mathbf{X}) \subset \mathbb{P} + \mathcal{F}_{K^{\mathbf{\Xi}}}(\mathbf{X}) \subset \mathcal{N}$.
From diagram (3.3), it comes

$$\forall f, g \in \mathcal{F}_{K,\mathbb{P}}, \ < f, g >_{\mathcal{F}_{K,\mathbb{P}}} =< (\mathrm{Id} - \boldsymbol{\pi}^{\mathbf{\Xi}})(f), (\mathrm{Id} - \boldsymbol{\pi}^{\mathbf{\Xi}})(g) >_{\mathcal{F}_{K^{\mathbf{\Xi}}}} =< f, g >_{\mathcal{N}} \ .$$

Hence $(\mathcal{F}_{K,\mathbb{P}}, <,>_{\mathcal{F}_{K,\mathbb{P}}})$ is a pre-hilbertian subspace of $\mathcal{N}$.
Let us now prove reproducing formula (4.7).
Let f be in $\mathcal{N}$ and $\mathbf{\Xi}' = \{\boldsymbol{\xi}_1', \ldots, \boldsymbol{\xi}_n'\}$ be a minimal $\mathbb{P}$-unisolvent set.
Observe first that:

$$< f, F_K(\delta_{\mathbf{x}}^{\mathbf{\Xi}'}) >_{\mathcal{N}} =< f - \boldsymbol{\pi}^{\mathbf{\Xi}}(f), F_K(\delta_{\mathbf{x}}^{\mathbf{\Xi}'}) - \boldsymbol{\pi}^{\mathbf{\Xi}}(F_K(\delta_{\mathbf{x}}^{\mathbf{\Xi}'})) >_{\mathcal{H}_{K^{\mathbf{\Xi}}}} \ .$$

From diagram (3.3), we get

$$F_K(\delta_{\mathbf{x}}^{\boldsymbol{\Xi}'}) - \boldsymbol{\pi}^{\boldsymbol{\Xi}}(F_K(\delta_{\mathbf{x}}^{\boldsymbol{\Xi}'})) = (\mathrm{Id} - \boldsymbol{\pi}^{\boldsymbol{\Xi}})(F_K(\delta_{\mathbf{x}}^{\boldsymbol{\Xi}'})) = F_{K^{\boldsymbol{\Xi}}}(\delta_{\mathbf{x}}^{\boldsymbol{\Xi}'})$$

and, since $\delta_{\mathbf{x}}^{\boldsymbol{\Xi}'} = \delta_{\mathbf{x}} - \sum_{k=1}^{n} h_k^{\boldsymbol{\Xi}'}(\mathbf{x})\delta_{\boldsymbol{\xi}'_k}$:

$$F_K(\delta_{\mathbf{x}}^{\boldsymbol{\Xi}'}) - \boldsymbol{\pi}^{\boldsymbol{\Xi}}(F_K(\delta_{\mathbf{x}}^{\boldsymbol{\Xi}'})) = K_{\mathbf{x}}^{\boldsymbol{\Xi}} - \sum_{k=1}^{n} h_k^{\boldsymbol{\Xi}'}(\mathbf{x}) K_{\boldsymbol{\xi}'_k}^{\boldsymbol{\Xi}}\,.$$

Hence, applying twice reproducing formula in $\mathcal{H}_{K^{\boldsymbol{\Xi}}}$,

$$\begin{aligned}
< f, F_K(\delta_{\mathbf{x}}^{\boldsymbol{\Xi}'}) >_{\mathcal{N}} &=< f - \boldsymbol{\pi}^{\boldsymbol{\Xi}}(f), K_{\mathbf{x}}^{\boldsymbol{\Xi}} - \sum_{k=1}^{n} h_k^{\boldsymbol{\Xi}'}(\mathbf{x}) K_{\boldsymbol{\xi}'_k}^{\boldsymbol{\Xi}} >_{\mathcal{H}_{K^{\boldsymbol{\Xi}}}} \\
&= f(\mathbf{x}) - \boldsymbol{\pi}^{\boldsymbol{\Xi}}(f)(\mathbf{x}) - \sum_{k=1}^{n} h_k^{\boldsymbol{\Xi}'}(\mathbf{x})(f(\boldsymbol{\xi}'_k) - \boldsymbol{\pi}^{\boldsymbol{\Xi}}(f)(\boldsymbol{\xi}'_k)) \\
&= f(\mathbf{x}) - \boldsymbol{\pi}^{\boldsymbol{\Xi}}(f)(\mathbf{x}) - \boldsymbol{\pi}^{\boldsymbol{\Xi}'}\left[f - \boldsymbol{\pi}^{\boldsymbol{\Xi}}(f)\right](\mathbf{x}) \\
&= f(\mathbf{x}) - \boldsymbol{\pi}^{\boldsymbol{\Xi}}(f)(\mathbf{x}) - \boldsymbol{\pi}^{\boldsymbol{\Xi}'}(f)(\mathbf{x}) + \boldsymbol{\pi}^{\boldsymbol{\Xi}'}(\boldsymbol{\pi}^{\boldsymbol{\Xi}}(f)(\mathbf{x}))
\end{aligned}$$

and eventually, as $\boldsymbol{\pi}^{\boldsymbol{\Xi}'} \circ \boldsymbol{\pi}^{\boldsymbol{\Xi}} = \boldsymbol{\pi}^{\boldsymbol{\Xi}}$

$$< f, F_K(\delta_{\mathbf{x}}^{\boldsymbol{\Xi}'}) >_{\mathcal{N}} = f(\mathbf{x}) - \boldsymbol{\pi}^{\boldsymbol{\Xi}'}(f)(\mathbf{x})$$

which is the reproducing formula (4.7).
□

4.2.3 General case: unicity

Lemma 4.4 *Let $\mathcal{N} \subset \mathbb{R}^E$ be satisfying properties of Theorem 4.1 and $\boldsymbol{\Xi} \subset E$ be a minimal $\mathbb{P}$-unisolvent set.*
Let us set $\overline{f}$ for the modulo $\mathbb{P}$ class of any $f \in \mathcal{N}$.
$\{\overline{K_{\mathbf{x}}^{\boldsymbol{\Xi}}} : \mathbf{x} \in E\}$ is a total set in the Hilbert space $\mathcal{N}/\mathbb{P}$.

Proof
Let $h \in \mathcal{N}$ be such that $\forall \mathbf{x} \in E,\ < \overline{h}, \overline{K_{\mathbf{x}}^{\boldsymbol{\Xi}}} >_{\mathcal{N}/\mathbb{P}} = 0$.
As $< \overline{h}, \overline{K_{\mathbf{x}}^{\boldsymbol{\Xi}}} >_{\mathcal{N}/\mathbb{P}} =< h, K_{\mathbf{x}}^{\boldsymbol{\Xi}} >_{\mathcal{N}}$, h satisfies

$$\forall \mathbf{x} \in E, < h, K_{\mathbf{x}}^{\boldsymbol{\Xi}} >_{\mathcal{N}} = 0$$

From reproducing property (4.7), we get, $\mathbf{x} \in E$:

$$h(\mathbf{x}) = \boldsymbol{\pi}^{\boldsymbol{\Xi}}(h)(\mathbf{x}) + < h, K_{\mathbf{x}}^{\boldsymbol{\Xi}} >_{\mathcal{N}} = \boldsymbol{\pi}^{\boldsymbol{\Xi}}(h)(\mathbf{x})$$

That is

$$h \in \mathbb{P} \text{ thus } \overline{h} = 0\,.$$

□
Suppose now that two spaces $\mathcal{N}, \mathcal{N}'$ satisfy theorem 4.1 specifications.
Let $\boldsymbol{\Xi}$ be a $\mathbb{P}$-unisolvent minimal set. From Lemma 4.4, it follows that both of

$\mathcal{N}/\mathbb{P}$ and $\mathcal{N}'/\mathbb{P}$ contain $\mathcal{F}_{K^{\Xi}}/\mathbb{P}$ as a dense subspace.
Hence identity function on $\mathcal{F}_{K^{\Xi}}/\mathbb{P}$ can be extended by an isometry

$$I : \mathcal{N}/\mathbb{P} \mapsto \mathcal{N}'/\mathbb{P}\,.$$

Thus, for any $\mathbf{x} \in E$ and $h \in \mathcal{N}$, applying again reproducing formula (4.7):

$$\begin{aligned} h(\mathbf{x}) &= \boldsymbol{\pi}^{\Xi}(h)(\mathbf{x}) + < h, K^{\Xi}_{\mathbf{x}} >_{\mathcal{N}} \\ &= \boldsymbol{\pi}^{\Xi}(h)(\mathbf{x}) + < \overline{h}, \overline{K^{\Xi}_{\mathbf{x}}} >_{\mathcal{N}/\mathbb{P}} \\ &= \boldsymbol{\pi}^{\Xi}(h)(\mathbf{x}) + < I(\overline{h}), I(\overline{K^{\Xi}_{\mathbf{x}}}) >_{\mathcal{N}'/\mathbb{P}} \\ &= \boldsymbol{\pi}^{\Xi}(h)(\mathbf{x}) + < h', K^{\Xi}_{\mathbf{x}} >_{\mathcal{N}'} \\ &= \boldsymbol{\pi}^{\Xi}(h)(\mathbf{x}) - \boldsymbol{\pi}^{\Xi}(h')(\mathbf{x}) + h'(\mathbf{x}) \end{aligned}$$

where $h' \in \mathcal{N}'$ is a class representant of $I(\overline{h})$.
So $h \in \mathcal{N}'$. $\square$

5 Interpolation in R.K.S.H.S

5.1 Preliminaries

In this section, we assume that

- $\mathbb{P}$ a finite dimensional vector space of functions.
- K is a $\mathbb{P}$-conditionally positive definite kernel
- $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset E$ is a $\mathbb{P}$-unisolvent set .

If we are given a minimal $\mathbb{P}$-unisolvent set $\boldsymbol{\Xi}$, we know that $\mathcal{F}_{K^{\Xi}}(\mathbf{X})$ is a (finite dimensional) vector subspace of Hilbert space $\mathcal{H}_{K^{\Xi}}$. By $[\mathcal{F}_{K^{\Xi}}(\mathbf{X})]^{\perp}$ is denoted the orthogonal complement of $\mathcal{F}_{K^{\Xi}}(\mathbf{X})$ in $\mathcal{H}_{K^{\Xi}}$.

5.2 Characterizations of interpolation in R.K.S.H.S

Let f be a function in $\mathcal{H}_{K,\mathbb{P}}$ that we only know on $\mathbf{X}$. We want to interpolate f in a reasonable way just using $f(\mathbf{x}_1), \ldots, f(\mathbf{x}_N)$ and K.
We start with a geometrical characterization of interpolation in $\mathcal{H}_{K,\mathbb{P}}$.

Proposition 5.1 *Let $\boldsymbol{\Xi} \subset \mathbf{X}$ be a minimal $\mathbb{P}$-unisolvent set.*
For every $f, g \in \mathcal{H}_{K,\mathbb{P}}$,

$$g \textit{ interpolates } f \textit{ on } \mathbf{X} \textit{ if and only if } f - g \in [\mathcal{F}_{K^{\Xi}}(\mathbf{X})]^{\perp}.$$

Proof
Applying reproducing property (4.7) to $f-g$, we get, for any $\mathbf{x} \in E$,

$$\begin{aligned} f(\mathbf{x}) - g(\mathbf{x}) &= \boldsymbol{\pi}^{\boldsymbol{\Xi}}(f-g)(\mathbf{x}) + < f-g, F_K(\delta_{\mathbf{x}}^{\boldsymbol{\Xi}}) >_{\mathcal{H}_{K,\mathbb{P}}} \\ &= \boldsymbol{\pi}^{\boldsymbol{\Xi}}(f-g)(\mathbf{x}) + < f-g-\boldsymbol{\pi}^{\boldsymbol{\Xi}}(f-g), F_K(\delta_{\mathbf{x}}^{\boldsymbol{\Xi}}) - \boldsymbol{\pi}^{\boldsymbol{\Xi}}(F_K(\delta_{\mathbf{x}}^{\boldsymbol{\Xi}})) >_{\mathcal{H}_{K^{\boldsymbol{\Xi}}}} . \end{aligned}$$

From diagram (3.3) comes:

$$F_K(\delta_{\mathbf{x}}^{\boldsymbol{\Xi}}) - \boldsymbol{\pi}^{\boldsymbol{\Xi}}(F_K(\delta_{\mathbf{x}}^{\boldsymbol{\Xi}})) = K_{\mathbf{x}}^{\boldsymbol{\Xi}} .$$

Hence

$$f(\mathbf{x}) - g(\mathbf{x}) = \boldsymbol{\pi}^{\boldsymbol{\Xi}}(f-g)(\mathbf{x}) + < f-g-\boldsymbol{\pi}^{\boldsymbol{\Xi}}(f-g), K_{\mathbf{x}}^{\boldsymbol{\Xi}} >_{\mathcal{H}_{K^{\boldsymbol{\Xi}}}} . \tag{5.1}$$

Suppose that g interpolates f on $\mathbf{X}$: $\forall \mathbf{x} \in \mathbf{X}, f(\mathbf{x}) = g(\mathbf{x})$.
Then, specifically,

$$\forall \boldsymbol{\xi} \in \boldsymbol{\Xi},\ f(\boldsymbol{\xi}) = g(\boldsymbol{\xi})$$

which means

$$\boldsymbol{\pi}^{\boldsymbol{\Xi}}(f) = \boldsymbol{\pi}^{\boldsymbol{\Xi}}(g)$$

and implies:

- $f - g \in \mathcal{H}_{K^{\boldsymbol{\Xi}}}$, from Proposition 4.2
- $0 = < f-g, K_{\mathbf{x}}^{\boldsymbol{\Xi}} >_{\mathcal{H}_{K^{\boldsymbol{\Xi}}}}, \forall \mathbf{x} \in \mathbf{X}$ from (5.1).

Hence, $f - g \in [\mathcal{F}_{K^{\boldsymbol{\Xi}}}(\mathbf{X})]^{\perp}$.
Conversely, if $f - g \in [\mathcal{F}_{K^{\boldsymbol{\Xi}}}(\mathbf{X})]^{\perp}$, then

$$\forall \mathbf{x} \in \mathbf{X},\ < f-g, K_{\mathbf{x}}^{\boldsymbol{\Xi}} >_{\mathcal{H}_{K^{\boldsymbol{\Xi}}}} = 0$$

which reads, by reproducing property in $\mathcal{H}_{K^{\boldsymbol{\Xi}}}$,

$$\forall \mathbf{x} \in \mathbf{X},\ f(\mathbf{x}) - \mathbf{g}(\mathbf{x}) = 0 .$$

□
From that proposition we draw this useful property

Corollary 5.1 *Any function f in $\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X})$ is uniquely defined by its value on $\mathbf{X}$.*

Proof
Suppose that $f, g \in \mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X})$ coincide on $\mathbf{X}$.
From Proposition 5.1 we know that $f - g \in [\mathcal{F}_{K^{\boldsymbol{\Xi}}}(\mathbf{X})]^{\perp}$.
And, according to (3.5) applied to $f-g$, we have $f - g \in \mathcal{F}_{K^{\boldsymbol{\Xi}}}(\mathbf{X})$.
Hence $f = g$.
□
We now state the main result about interpolation: among all the interpolators lying in $\mathcal{H}_{K,\mathbb{P}}$ of any function $f \in \mathcal{H}_{K,\mathbb{P}}$ on $\mathbf{X}$, the *best* one belongs to $\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X})$. That comes out from:

Proposition 5.2 *Let f be in $\mathcal{H}_{K,\mathbb{P}}$.*
If $\mathbf{X}$ is $\mathbb{P}$-unisolvent,

1. *The following problem*
$$\min_{g\in\mathbb{P}+\mathcal{F}_{K,\mathbb{P}}(\mathbf{X})} ||f-g||_{\mathcal{H}_{K,\mathbb{P}}} \tag{5.2}$$
has a unique solution which interpolates f *on* $\mathbf{X}$*. Let* $S_{K,\mathbb{P},\mathbf{X}}(f)$ *denote this interpolator.*

2. *Given a minimal* $\mathbb{P}$*-unisolvent set* $\boldsymbol{\Xi}\subset\mathbf{X}$*,*
$$S_{K,\mathbb{P},\mathbf{X}}(f)=\boldsymbol{\pi}^{\boldsymbol{\Xi}}(f)+S_{K^{\boldsymbol{\Xi}},\mathbf{X}}(f-\boldsymbol{\pi}^{\boldsymbol{\Xi}}(f)) \tag{5.3}$$
where $S_{K^{\boldsymbol{\Xi}},\mathbf{X}}:\mathcal{H}_{K^{\boldsymbol{\Xi}}}\mapsto\mathcal{F}_{K^{\boldsymbol{\Xi}}}(\mathbf{X})$ *denotes the orthogonal projector on* $\mathcal{F}_{K^{\boldsymbol{\Xi}}}(\mathbf{X})$ *.*

3. $S_{K,\mathbb{P},\mathbf{X}}(f)$ *is the interpolator of* f *on* $\mathbf{X}$ *with minimal semi-norm.*

Proof

Let $\boldsymbol{\Xi}$ be any $\mathbb{P}$-unisolvent set and g be defined as
$$g=\boldsymbol{\pi}^{\boldsymbol{\Xi}}(f)+S_{K^{\boldsymbol{\Xi}},\mathbf{X}}(f-\boldsymbol{\pi}^{\boldsymbol{\Xi}}(f))$$
which is meaningful since $f-\boldsymbol{\pi}^{\boldsymbol{\Xi}}(f)\in\mathcal{H}_{K^{\boldsymbol{\Xi}}}$.
We have, $S_{K^{\boldsymbol{\Xi}},\mathbf{X}}$ being the orthogonal projection on $\mathcal{F}_{K^{\boldsymbol{\Xi}}}(\mathbf{X})$:
$$f-g=f-\boldsymbol{\pi}^{\boldsymbol{\Xi}}(f)-S_{K^{\boldsymbol{\Xi}},\mathbf{X}}(f-\boldsymbol{\pi}^{\boldsymbol{\Xi}}(f))\in[\mathcal{F}_{K^{\boldsymbol{\Xi}}}(\mathbf{X})]^{\perp}\ .$$
Hence, from Proposition 5.1 it follows that g interpolates f on $\mathbf{X}$.
Besides, by construction g lies in $\mathbb{P}+\mathcal{F}_{K^{\boldsymbol{\Xi}}}(\mathbf{X})$ and, recalling (3.6):
$$\mathbb{P}+\mathcal{F}_{K,\mathbb{P}}(\mathbf{X})=\mathbb{P}+\mathcal{F}_{K^{\boldsymbol{\Xi}}}(\mathbf{X})$$
g lies $\mathbb{P}+\mathcal{F}_{K,\mathbb{P}}(\mathbf{X})$.
Now, let us recall this easy fact, for two any functions φ_1,φ_2, belonging to $\mathcal{H}_{K,\mathbb{P}}$:
$$||\varphi_1-\varphi_2||^2_{\mathcal{H}_{K,\mathbb{P}}}=||\varphi_1-g+g-\varphi_2||^2_{\mathcal{H}_{K,\mathbb{P}}}=||\varphi_1-g||^2_{\mathcal{H}_{K,\mathbb{P}}}+||g-\varphi_2||^2_{\mathcal{H}_{K,\mathbb{P}}}+2<\varphi_1-g,g-\varphi_2>_{\mathcal{H}_{K,\mathbb{P}}}\ . \tag{5.4}$$
Let $h\in\mathbb{P}+\mathcal{F}_{K,\mathbb{P}}(\mathbf{X})=\mathbb{P}+\mathcal{F}_{K^{\boldsymbol{\Xi}}}(\mathbf{X})$.
Applying (5.4) to $\varphi_1=f$ and $\varphi_2=h$ leads to
$$||f-h||^2_{\mathcal{H}_{K,\mathbb{P}}}=||f-g||^2_{\mathcal{H}_{K,\mathbb{P}}}+||g-h||^2_{\mathcal{H}_{K,\mathbb{P}}}+2<f-g,g-h>_{\mathcal{H}_{K,\mathbb{P}}}\ . \tag{5.5}$$
Since
$$g-h-\boldsymbol{\pi}^{\boldsymbol{\Xi}}(g-h)\in\mathcal{F}_{K^{\boldsymbol{\Xi}}}(\mathbf{X})$$
and, $f-g\in[\mathcal{F}_{K^{\boldsymbol{\Xi}}}(\mathbf{X})]^{\perp}$, then
$$<f-g,g-h>_{\mathcal{H}_{K,\mathbb{P}}}=<f-g,g-h-\boldsymbol{\pi}^{\boldsymbol{\Xi}}(g-h)>_{\mathcal{H}_{K^{\boldsymbol{\Xi}}}}=0\,.$$
Thus, relation (5.5) gives:
$$||f-h||^2_{\mathcal{H}_{K,\mathbb{P}}}=||f-g||^2_{\mathcal{H}_{K,\mathbb{P}}}+||g-h||^2_{\mathcal{H}_{K,\mathbb{P}}}.$$

That shows that g is a solution of problem (5.2). By corollary 5.1 there is no other interpolant of f in $\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X})$.
Let now $h \in \mathcal{H}_{K,\mathbb{P}}$ be an other interpolator of f on $\mathbf{X}$. Let us apply (5.4) to $\varphi_1 = h$, and $\varphi_2 = 0$:

$$||h||^2_{\mathcal{H}_{K,\mathbb{P}}} = ||h-g||^2_{\mathcal{H}_{K,\mathbb{P}}} + ||g||^2_{\mathcal{H}_{K,\mathbb{P}}} + 2 < h-g, g >_{\mathcal{H}_{K,\mathbb{P}}} . \tag{5.6}$$

Since h interpolates f on $\mathbf{X}$, it also interpolates g on $\mathbf{X}$. Proposition 5.1 tells us that

$$h - g \in [\mathcal{F}_{K^{\mathbf{\Xi}}}(\mathbf{X})]^{\perp} .$$

Hence, since $g - \boldsymbol{\pi}^{\mathbf{\Xi}}(g) \in \mathcal{F}_{K^{\mathbf{\Xi}}}(\mathbf{X})$

$$< h-g, g >_{\mathcal{H}_{K,\mathbb{P}}} = < h-g, g - \boldsymbol{\pi}^{\mathbf{\Xi}}(g) >_{\mathcal{H}_{K^{\mathbf{\Xi}}}} = 0 .$$

Relation (5.6) becomes

$$||h||^2_{\mathcal{H}_{K,\mathbb{P}}} = ||h-g||^2_{\mathcal{H}_{K,\mathbb{P}}} + ||g||^2_{\mathcal{H}_{K,\mathbb{P}}} .$$

Thus, $||h||_{\mathcal{H}_{K,\mathbb{P}}} \geq ||g||_{\mathcal{H}_{K,\mathbb{P}}}$.
Moreover, $||h||_{\mathcal{H}_{K,\mathbb{P}}} = ||g||_{\mathcal{H}_{K,\mathbb{P}}}$ only when $||h-g||_{\mathcal{H}_{K,\mathbb{P}}} = 0$. Since h interpolates g on $\mathbf{X}$, hence on $\mathbf{\Xi}$, we have $\boldsymbol{\pi}^{\mathbf{\Xi}}(h-g) = 0$ and

$$||h-g||_{\mathcal{H}_{K,\mathbb{P}}} = 0 \Leftrightarrow ||h-g-\boldsymbol{\pi}^{\mathbf{\Xi}}(h-g)||_{\mathcal{H}_{K^{\mathbf{\Xi}}}} = 0 \Leftrightarrow ||h-g||_{\mathcal{H}_{K^{\mathbf{\Xi}}}} = 0 \Leftrightarrow h = g .$$

□

5.3 Lagrangian form of R.K.S.H.S interpolators

We now want to set in our framework, the formulation known as Lagrangian formulation ([6], [11]), which is much better for error analysis.
We first introduce a useful tool.

5.3.1 Free $\mathbb{P}$-unisolvent set

Definition 5.1 *Any $\mathbb{P}$-unisolvent set $\mathbf{Z}$ which does not possess a strict $\mathbb{P}$-unisolvent subset $\mathbf{Y}$ satisfying*

$$\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z}) = \mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Y})$$

*will be called a (K-)***free** *$\mathbb{P}$-unisolvent set.*

We will state two characterizations of freeness.
The first one is:

Lemma 5.1 *A $\mathbb{P}$-unisolvent set $\mathbf{Z}$ is a free $\mathbb{P}$-unisolvent set if and only if*

$$\dim(\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z})) = \mathrm{Cardinal}(\mathbf{Z}) .$$

Proof
Suppose that $\mathbf{Z}$ is free.
If $\mathbf{Z}$ is a minimal $\mathbb{P}$-unisolvent set, we have Cardinal$(\mathbf{Z}) = n$ and $\mathcal{M}_{\mathbb{P}}(\mathbf{Z}) = \{0\}$. Hence $\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z}) = \mathbb{P}$ and

$$\dim(\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z})) = \text{Cardinal}(\mathbf{Z})\,.$$

Now, if $\mathbf{Z}$ is not a minimal $\mathbb{P}$-unisolvent set, it strictly contains a minimal $\mathbb{P}$-unisolvent set $\mathbf{\Xi}$.
Let us first show that $K^{\mathbf{\Xi}}_{\mathbf{z}}, \mathbf{z} \in \mathbf{Z} - \mathbf{\Xi}$ is a $\mathcal{F}_{K^{\mathbf{\Xi}}}(\mathbf{Z})$-basis.
Otherwise there would be $\mathbf{z}_0 \in \mathbf{Z} - \mathbf{\Xi}$ such that, setting $\mathbf{Z}' = \mathbf{Z} - \{\mathbf{z}_0\}$, $K^{\mathbf{\Xi}}_{\mathbf{z}}, \mathbf{z} \in \mathbf{Z}' - \mathbf{\Xi}$ spans $\mathcal{F}_{K^{\mathbf{\Xi}}}(\mathbf{Z})$. Hence we would have $\mathbb{P} + \mathcal{F}_{K^{\mathbf{\Xi}}}(\mathbf{Z}') = \mathbb{P} + \mathcal{F}_{K^{\mathbf{\Xi}}}(\mathbf{Z})$ or equivalently

$$\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z}') = \mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z})$$

which, since $\mathbf{Z}'$, containing $\mathbf{\Xi}$, is a $\mathbb{P}$- unisolvent set, conflicts with $\mathbf{Z}$ beeing free.
Therefore $\dim(\mathbb{P}+\mathcal{F}_{K,\mathbb{P}}(\mathbf{Z})) = \dim(\mathbb{P}+\mathcal{F}_{K^{\mathbf{\Xi}}}(\mathbf{Z})) = n + \text{Cardinal}(\mathbf{Z}) - n = \text{Cardinal}(\mathbf{Z})$.
Conversely assume that $\dim(\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z})) = \text{Cardinal}(\mathbf{Z})$.
If $\mathbf{Z}$ were not free. There would exist $\mathbf{Z}'$, a $\mathbb{P}$-unisolvent strict subset of $\mathbf{Z}$, verifying

$$\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z}') = \mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z})\,.$$

Thus, since $K^{\mathbf{\Xi}}_{\mathbf{z}}, \mathbf{z} \in \mathbf{Z}' - \mathbf{\Xi}$ spans $\mathcal{F}_{K^{\mathbf{\Xi}}}(\mathbf{Z}')$:

$$\dim(\mathbb{P}+\mathcal{F}_{K,\mathbb{P}}(\mathbf{Z})) = \dim(\mathbb{P}+\mathcal{F}_{K,\mathbb{P}}(\mathbf{Z}')) = \dim(\mathbb{P}) + \dim(\mathcal{F}_{K^{\mathbf{\Xi}}}(\mathbf{Z}')) < n + \text{Cardinal}(\mathbf{Z}) - n = \text{Cardinal}(\mathbf{Z})$$

which conficts with the hypothesis $\dim(\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z})) = \text{Cardinal}(\mathbf{Z})$. $\square$
In order to state our second freeness characterization, we need some more definitions.

Definition 5.2 *Let $\mathcal{P} = (p_1, \dots, p_n)$ be a $\mathbb{P}$-basis.*
To any finite set $\mathbf{Z} = \{\mathbf{z}_1, \dots, \mathbf{z}_M\} \subset E$ we define the matrix

$$\mathbf{Q}_{\mathcal{P},\mathbf{Z}} = \begin{pmatrix} \mathbf{K}_{\mathbf{Z}} & \mathbf{P}_{\mathbf{Z}} \\ {\mathbf{P}_{\mathbf{Z}}}^T & 0 \end{pmatrix}$$

where

- $\mathbf{P}_{\mathbf{Z}} = \begin{pmatrix} p_1(\mathbf{z}_1) & \dots & p_n(\mathbf{z}_1) \\ \vdots & \dots & \vdots \\ p_1(\mathbf{z}_M) & \dots & p_n(\mathbf{z}_M) \end{pmatrix}$
- $\mathbf{K}_{\mathbf{Z}} = \begin{pmatrix} K(\mathbf{z}_1, \mathbf{z}_1) & \dots & K(\mathbf{z}_1, \mathbf{z}_M) \\ \vdots & \dots & \vdots \\ K(\mathbf{z}_M, \mathbf{z}_1) & \dots & K(\mathbf{z}_M, \mathbf{z}_M) \end{pmatrix}.$

If $\mathbf{Q}_{\mathcal{P},\mathbf{Z}}$ is non degenerate we have this helpful construction.

Lemma 5.2 *$\mathcal{P}$ and $\mathbf{Z}$ being as in definition 5.2, if $\mathbf{Q}_{\mathcal{P},\mathbf{Z}}$ is non degenerate the application $\mathcal{R}_{\mathcal{P},\mathbf{Z}}$ defined as*

$$\mathcal{R}_{\mathcal{P},\mathbf{Z}} : \mathbf{w} \in \mathbb{R}^M \mapsto \sum_{i=1}^{n} \alpha_i(\mathbf{w}) p_i + \sum_{j=1}^{M} \gamma_j(\mathbf{w}) K_{\mathbf{z}_j}$$

where, for any $\mathbf{w} \in \mathbb{R}^M$, $\boldsymbol{\alpha}(\mathbf{w}) = \begin{pmatrix} \alpha_1(\mathbf{w}) \\ \vdots \\ \alpha_n(\mathbf{w}) \end{pmatrix} \in \mathbb{R}^n$, $\boldsymbol{\gamma}(\mathbf{w}) = \begin{pmatrix} \gamma_1(\mathbf{w}) \\ \vdots \\ \gamma_M(\mathbf{w}) \end{pmatrix} \in \mathbb{R}^M$ *are such that* $\begin{pmatrix} \boldsymbol{\gamma}(\mathbf{w}) \\ \boldsymbol{\alpha}(\mathbf{w}) \end{pmatrix} = \mathbf{Q}_{\mathcal{P},\mathbf{Z}}^{-1} \begin{pmatrix} \mathbf{w} \\ 0 \end{pmatrix}$ *is a linear isomorphism between* $\mathbb{R}^M$ *and* $\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z})$.

Proof

For any $\mathbf{w} \in \mathbb{R}^M$,

$$\begin{pmatrix} \boldsymbol{\gamma}(\mathbf{w}) \\ \boldsymbol{\alpha}(\mathbf{w}) \end{pmatrix} = \mathbf{Q}_{\mathcal{P},\mathbf{Z}}^{-1} \begin{pmatrix} \mathbf{w} \\ 0 \end{pmatrix}$$

is equivalently rephrased as

$$(\boldsymbol{\alpha}(\mathbf{w}), \boldsymbol{\gamma}(\mathbf{w})) \text{ is the unique solution of } \left\{ \begin{array}{cccc} \mathbf{K_Z}\boldsymbol{\gamma} & + & \mathbf{P_Z}\boldsymbol{\alpha} & = & \mathbf{w} \\ \mathbf{P_Z}^T\boldsymbol{\gamma} & & & = & 0 \end{array} \right. .$$

The second equation tells us that $\mathcal{R}_{\mathcal{P},\mathbf{Z}}(\mathbf{w}) = \sum_{i=1}^n \alpha_i(\mathbf{w})p_i + \sum_{j=1}^M \gamma_j(\mathbf{w})K_{\mathbf{z}_j} \in \mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z})$. Moreover, $\mathcal{R}_{\mathcal{P},\mathbf{Z}}$ is an onto application since if $g = \sum_{i=1}^n \alpha_i p_i + \sum_{j=1}^M \gamma_j K_{\mathbf{z}_j} \in \mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z})$, let $g_\mathbf{Z}$ be the vector whose coordinates are the values taken by g on $\mathbf{Z}$, we have

$$\left\{ \begin{array}{cccc} \mathbf{K_Z}\boldsymbol{\gamma} & + & \mathbf{P_Z}\boldsymbol{\alpha} & = & g_\mathbf{Z} \\ \mathbf{P_Z}^T\boldsymbol{\gamma} & & & = & 0 \end{array} \right.$$

which means $\mathcal{R}_{\mathcal{P},\mathbf{Z}}(g_\mathbf{Z}) = g$.

Lastly, $\mathcal{R}_{\mathcal{P},\mathbf{Z}}$ is injective, since, according to corollary 5.1, $\mathcal{R}_{\mathcal{P},\mathbf{Z}}(\mathbf{w})$ as a function of $\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z})$ is uniquely defined by its values on $\mathbf{Z}$, which are the coordinates of $\mathbf{w}$.

Therafter $\mathcal{R}_{\mathcal{P},\mathbf{Z}}$ is a bijection from $\mathbb{R}^M$ to $\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z})$. $\square$

We can then state our second freeness characterization

Lemma 5.3 *Let* $\mathcal{P}$ *be a* $\mathbb{P}$*-basis.*
A $\mathbb{P}$*-unisolvent set* $\mathbf{Z}$ *is free if and only if* $\mathbf{Q}_{\mathcal{P},\mathbf{Z}}$ *is non degenerate.*

Proof

Let us denote $M = \text{Cardinal}(\mathbf{Z})$.

Suppose that $\mathbf{Q}_{\mathcal{P},\mathbf{Z}}$ is degenerate: let $(\boldsymbol{\gamma}, \boldsymbol{\alpha}) \neq (0,0) \in \mathbb{R}^n \times \mathbb{R}^M$ such that $\mathbf{Q}_{\mathcal{P},\mathbf{Z}} \begin{pmatrix} \boldsymbol{\gamma} \\ \boldsymbol{\alpha} \end{pmatrix} = 0$ i.e

$$\left\{ \begin{array}{cccc} \mathbf{K_Z}\boldsymbol{\gamma} & + & \mathbf{P_Z}\boldsymbol{\alpha} & = & 0 \\ \mathbf{P_Z}^T\boldsymbol{\gamma} & & & = & 0 \end{array} \right. . \tag{5.7}$$

The function $f = \sum_{i=1}^n \alpha_i p_i + \sum_{j=1}^M \gamma_j K_{\mathbf{z}_j}$ is in $\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z})$ since the second equation of (5.7) implies $\sum_{j=1}^M \gamma_j \delta_{\mathbf{z}_j} \in \mathcal{M}_\mathbb{P}(\mathbf{Z})$. The first equation tells us that f is null on $\mathbf{Z}$, and actually everywhere from corollary 5.1 of Proposition 5.1.

Now

$$f = 0 \Leftrightarrow \sum_{i=1}^n \alpha_i p_i = -\sum_{j=1}^M \gamma_j K_{\mathbf{z}_j} .$$

But that implies

$$\begin{cases} \sum_{i=1}^n \alpha_i p_i = 0 \\ \sum_{j=1}^M \gamma_j K_{\mathbf{z}_j} = 0 \end{cases} \tag{5.8}$$

since, K being $\mathbb{P}$-conditionally positive definite, we have $\mathbb{P} \cap \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z}) = \{0\}$.
First equation of (5.8) gives $\alpha_i = 0, i = 1, \ldots, n$, since $\mathcal{P} = \{p_1, \ldots, p_n\}$ is a $\mathbb{P}$-basis.
Hence

$$\sum_{j=1}^M \gamma_j K_{\mathbf{z}_j} = 0 \tag{5.9}$$

with at least one of the $\gamma_j, j = 1, \ldots, M$ being different of 0.
Notice that consequently, $\mathbf{Z}$ which is $\mathbb{P}$-unisolvent cannot be a **minimal** $\mathbb{P}$-unisolvent set: if it were then $\mathcal{M}_{\mathbb{P}}(\mathbf{Z}) = \{0\}$ and therefore $\sum_{j=1}^M \gamma_j \delta_{\mathbf{z}_j} = 0$. That would imply that $\gamma_j = 0, j = 1, \ldots, M$.
So $\mathbf{Z}$ contains a minimal $\mathbb{P}$-unisolvent set $\mathbf{\Xi}$ which is a strict subset. Observe, now, that at least one l of $\{1, \ldots, M\}$ is such that $\mathbf{z}_l \in \mathbf{Z} - \mathbf{\Xi}$ and $\gamma_l \neq 0$: otherwise, $\sum_{j=1}^M \gamma_j \delta_{\mathbf{z}_j}$ would belong to $\mathcal{M}_{\mathbb{P}}(\mathbf{\Xi})$ which reduces to $\{0\}$ and therefore $\gamma_j = 0, j = 1, \ldots, M$ would be implied.
Thus, there is j, say $j = 1$, such that $\mathbf{Z}' = \mathbf{Z} - \{\mathbf{z}_1\}$ is $\mathbb{P}$-unisolvent and $\gamma_1 \neq 0$.
Let us now show that $\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z}) = \mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z}')$.
Thanks to (5.9), every $g = \sum_{i=1}^n \beta_i p_i + \sum_{j=1}^M \rho_j K_{\mathbf{z}_j}$ in $\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z})$ can be written

$$g = \sum_{i=1}^n \beta_i p_i + \sum_{j=2}^M (\rho_j - \rho_1 \frac{\gamma_j}{\gamma_1}) K_{\mathbf{z}_j} \,.$$

To show that $g \in \mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z}')$ we just have to verify that: $\sum_{j=2}^M (\rho_j - \rho_1 \frac{\gamma_j}{\gamma_1}) \delta_{\mathbf{z}_j} \in \mathcal{M}_{\mathbb{P}}$.
Indeed, for $p \in \mathbb{P}$

$$\begin{aligned} \sum_{j=2}^M (\rho_j - \rho_1 \frac{\gamma_j}{\gamma_1}) p(\mathbf{z}_j) &= \sum_{j=2}^M \rho_j p(\mathbf{z}_j) - \frac{\rho_1}{\gamma_1} \sum_{j=2}^M \gamma_j p(\mathbf{z}_j) \\ &= -\rho_1 p(\mathbf{z}_1) + \frac{\rho_1}{\gamma_1} \gamma_1 p(\mathbf{z}_1) \\ &= 0 \end{aligned}$$

where we used

$$\sum_{j=1}^M \rho_j \delta_{\mathbf{z}_j} \in \mathcal{M}_{\mathbb{P}} \Rightarrow \sum_{j=1}^M \rho_j p(\mathbf{z}_j) = 0 \Rightarrow \sum_{j=2}^M \rho_j p(\mathbf{z}_j) = -\rho_1 p(\mathbf{z}_1)$$

and

$$\sum_{j=1}^M \gamma_j \delta_{\mathbf{z}_j} \in \mathcal{M}_{\mathbb{P}} \Rightarrow \sum_{j=1}^M \gamma_j p(\mathbf{z}_j) = 0 \Rightarrow \sum_{j=2}^M \gamma_j p(\mathbf{z}_j) = -\gamma_1 p(\mathbf{z}_1) \,.$$

Conversely, if $\mathbf{Q}_{\mathcal{P},\mathbf{Z}}$ is not degenerate, then from Lemma 5.2, we know that $\mathcal{R}_{\mathcal{P},\mathbf{Z}}$ is a linear isomorphism between $\mathbb{R}^M$ and $\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z})$ and we thus have:

$$\dim(\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{Z})) = \mathrm{Cardinal}(\mathbf{Z})$$

which from Lemma 5.1 implies that $\mathbf{Z}$ is free. □

5.3.2 Lagrangian formulation

Proposition 5.3 (Lagrangian formulation) *Let $\mathbf{X}$ be a $\mathbb{P}$-unisolvent set. For any free $\mathbb{P}$-unisolvent set $\mathbf{X}' = \{\mathbf{x}'_1, \ldots, \mathbf{x}'_{N'}\} \subset \mathbf{X}$ satisfying*

$$\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X}) = \mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X}') \tag{5.10}$$

the following relations uniquely define $u_1, \ldots, u_{N'}$ in $\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X})$

$$u_k(\mathbf{x}'_l) = \delta_{k,l}, \forall k, l \in \{1, \ldots, N'\}. \tag{5.11}$$

Moreover $u_1, \ldots, u_{N'}$ is a $[\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X})]$-basis, and every $g \in \mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X})$ can be written

$$g = \sum_{k=1}^{N'} g(\mathbf{x}'_k) u_k. \tag{5.12}$$

Consequently

$$\forall f \in \mathcal{H}_{K,\mathbb{P}},\ S_{K,\mathbb{P},\mathbf{X}}(f) = \sum_{k=1}^{N'} f(\mathbf{x}'_k) u_k. \tag{5.13}$$

Proof
Let $\mathbf{X}' = \{\mathbf{x}'_1, \ldots, \mathbf{x}'_{N'}\}$ be a free $\mathbb{P}$-unisolvent subset of $\mathbf{X}$, such that $\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X}) = \mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X}')$ and $\mathcal{P}$ be a $\mathbb{P}$-basis.
The application $\mathcal{R}_{\mathcal{P},\mathbf{X}'}$ defined in Lemma 5.2 is a linear isomorphism between $\mathbb{R}^{N'}$ and $\mathbb{P} + \mathcal{F}_K(\mathbf{X}') = \mathbb{P} + \mathcal{F}_K(\mathbf{X})$.
Let $\mathbf{e}_1, \ldots, \mathbf{e}_{N'}$ be the canonical $\mathbb{R}^{N'} - basis$.
Let us set:

$$u_j = \mathcal{R}_{\mathcal{P},\mathbf{X}'}(\mathbf{e}_j)$$

where $u_1, \ldots, u_{N'}$ satisfies (5.11).
Indeed, $u_k = \mathcal{R}_{\mathcal{P},\mathbf{X}'}(\mathbf{e}_k)$ means:

$$u_k = \sum_{i=1}^{n} \alpha_i^{(k)} p_i + \sum_{j=1}^{N'} \gamma_j^{(k)} K_{\mathbf{x}'_j}$$

where $\boldsymbol{\alpha}^{(k)} = \begin{pmatrix} \alpha_1^{(k)} \\ \vdots \\ \alpha_n^{(k)} \end{pmatrix}$, $\boldsymbol{\gamma}^{(k)} = \begin{pmatrix} \gamma_1^{(k)} \\ \vdots \\ \gamma_{N'}^{(k)} \end{pmatrix}$ is the unique solution of

$$\left\{ \begin{array}{lclcl} \mathbf{K}_{\mathbf{X}'}\boldsymbol{\gamma} & + & \mathbf{P}_{\mathbf{X}'}\boldsymbol{\alpha} & = & \mathbf{e}_k \\ \mathbf{P}_{\mathbf{X}'}{}^T\boldsymbol{\gamma} & & & = & 0 \end{array} \right. . \tag{5.14}$$

The first equation reads exactly: $u_k(\mathbf{z}_l) = \left\{ \begin{array}{l} 0 \text{ if } k \neq l \\ 1 \text{ if } k = l \end{array} \right.$ which is (5.11).
Now, satisfying (5.11), $u_1, \ldots, u_{N'}$ are obviously linearly independant, and, since

$$N' = \dim(\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X}')) = \dim(\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X}))$$

$u_1, \ldots, u_{N'}$ is a $[\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X})]$-basis.
Every $g \in \mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X})$ can thus be written $g = \sum_{i=1}^{N'} \alpha_i u_i$, and by (5.11) we get

$$g(\mathbf{x}'_j) = \sum_{i=1}^{N'} \alpha_i u_i(\mathbf{x}'_j) = \alpha_j$$

hence (5.12).
And (5.13) follows immediately.
Unicity of $u_1, \ldots, u_{N'}$ satisfying (5.11) is immediate, since any other $v_1, \ldots, v_{N'}$ satisfying (5.11) would verify

$$v_j = \sum_{i=1}^{N'} v_i(\mathbf{x}'_j) u_i = u_j \, .$$

□
To conclude this section devoted to interpolation, let us make three remarks

1. The preceding proof gives a direct mean to compute $(u_1, \ldots, u_{N'})$: we only have to solve (5.14), that is to compute the inverse of $\mathbf{Q}_{\mathcal{P},\mathbf{X}'}$.

2. In the native spaces and kriging literature ([6], or [11]), we find this relation:
$$\left\{ \begin{array}{lllll} \mathbf{K}_{\mathbf{X}'} \; \mathbf{u}(\mathbf{x}) & + & \mathbf{P}_{\mathbf{X}'} \; \mathbf{v}(\mathbf{x}) & = & \mathbf{k}_{\mathbf{X}'}(\mathbf{x}) \\ {\mathbf{P}_{\mathbf{X}'}}^T \; \mathbf{u}(\mathbf{x}) & & & = & \mathbf{p}(\mathbf{x}) \end{array} \right. \tag{5.15}$$
satisfied by $\mathbf{k}_{\mathbf{X}'}(\mathbf{x}) = \begin{pmatrix} K_{\mathbf{x}'_1}(\mathbf{x}) \\ \vdots \\ K_{\mathbf{x}'_{N'}}(\mathbf{x}) \end{pmatrix}$, $\mathbf{p}(\mathbf{x}) = \begin{pmatrix} p_1(\mathbf{x}) \\ \vdots \\ p_n(\mathbf{x}) \end{pmatrix}$, $\mathbf{u}(\mathbf{x}) = \begin{pmatrix} u_1(\mathbf{x}) \\ \vdots \\ u_{N'}(\mathbf{x}) \end{pmatrix}$
and a vector $\mathbf{v}(\mathbf{x}) = \begin{pmatrix} v_1(\mathbf{x}) \\ \vdots \\ v_{N'}(\mathbf{x}) \end{pmatrix} \in \mathbb{R}^n$.
The resolution of (5.15) in $\mathbf{u}(\mathbf{x}), \mathbf{v}(\mathbf{x})$ leads to $u_1(\mathbf{x}), \ldots, u_{N'}(\mathbf{x})$.
Let us see why there exists $\mathbf{v}(\mathbf{x}) \in \mathbb{R}^n$ such that (5.15) is verified.
Firstly, each of $(p_1, \ldots, p_n)$ beeing in $\mathbb{P}$ belongs to $\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X}')$. Thus

$$p_i(\mathbf{x}) = \sum_{k=1}^{N'} p_i(\mathbf{x}_k) u_k(\mathbf{x}), i = 1, \ldots, n$$

which is the second equation of (5.15).
Then, recall that

$$u_k(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i^{(k)} p_i(\mathbf{x}) + \sum_{j=1}^{N'} \gamma_j^{(k)} K_{\mathbf{x}'_j}(\mathbf{x}) = \begin{pmatrix} \boldsymbol{\gamma}^{(k)T} & \boldsymbol{\alpha}^{(k)T} \end{pmatrix} \begin{pmatrix} \mathbf{k}_{\mathbf{X}'}(\mathbf{x}) \\ \mathbf{p}(\mathbf{x}) \end{pmatrix}$$

where $\boldsymbol{\alpha}^{(k)} = \begin{pmatrix} \alpha_1^{(k)} \\ \vdots \\ \alpha_n^{(k)} \end{pmatrix}$, $\boldsymbol{\gamma}^{(k)} = \begin{pmatrix} \gamma_1^{(k)} \\ \vdots \\ \gamma_{N'}^{(k)} \end{pmatrix}$ are given by
$\begin{pmatrix} \boldsymbol{\gamma}^{(k)} \\ \boldsymbol{\alpha}^{(k)} \end{pmatrix} = \mathbf{Q}_{\mathcal{P},\mathbf{X}'}^{-1} \begin{pmatrix} \mathbf{e}_k \\ 0 \end{pmatrix}$ so that:

$$\mathbf{u}(\mathbf{x}) = \begin{pmatrix} {\boldsymbol{\gamma}^{(1)}}^T & {\boldsymbol{\alpha}^{(1)}}^T \\ \vdots & \vdots \\ {\boldsymbol{\gamma}^{(N')}}^T & {\boldsymbol{\alpha}^{(N')}}^T \end{pmatrix} \begin{pmatrix} \mathbf{k}_{\mathbf{X}'}(\mathbf{x}) \\ \mathbf{p}(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} \mathrm{Id}_{N'} & 0 \end{pmatrix} \mathbf{Q}_{\mathcal{P},\mathbf{X}'}^{-1} \begin{pmatrix} \mathbf{k}_{\mathbf{X}'}(\mathbf{x}) \\ \mathbf{p}(\mathbf{x}) \end{pmatrix}$$

and

$$\mathbf{K}_{\mathbf{X}'}\mathbf{u}(\mathbf{x}) = \mathbf{K}_{\mathbf{X}'} \begin{pmatrix} \mathrm{Id}_{N'} & 0 \end{pmatrix} \mathbf{Q}_{\mathcal{P},\mathbf{X}'}^{-1} \begin{pmatrix} \mathbf{k}_{\mathbf{X}'}(\mathbf{x}) \\ \mathbf{p}(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} \mathbf{K}_{\mathbf{X}'} & 0 \end{pmatrix} \mathbf{Q}_{\mathcal{P},\mathbf{X}'}^{-1} \begin{pmatrix} \mathbf{k}_{\mathbf{X}'}(\mathbf{x}) \\ \mathbf{p}(\mathbf{x}) \end{pmatrix}.$$

Now it is readily seen that

$$\begin{pmatrix} \mathbf{K}_{\mathbf{X}'} & 0 \end{pmatrix} \mathbf{Q}_{\mathcal{P},\mathbf{X}'}^{-1} = \begin{pmatrix} \mathrm{Id}_{N'} & 0 \end{pmatrix} - \mathbf{P}_{\mathbf{X}'}\mathbf{M} \tag{5.16}$$

for a $(n \times (N'+n))$ well chosen matrix $\mathbf{M}$, leading to

$$\mathbf{K}_{\mathbf{X}'}\mathbf{u}(\mathbf{x}) + \mathbf{P}_{\mathbf{X}'}\mathbf{M} \begin{pmatrix} \mathbf{k}_{\mathbf{X}'}(\mathbf{x}) \\ \mathbf{p}(\mathbf{x}) \end{pmatrix} = \mathbf{k}_{\mathbf{X}'}(\mathbf{x})$$

which is the first equation of (5.15) with $\mathbf{v}(\mathbf{x}) = \mathbf{M} \begin{pmatrix} \mathbf{k}_{\mathbf{X}'}(\mathbf{x}) \\ \mathbf{p}(\mathbf{x}) \end{pmatrix}$.
Regarding (5.16), let us denote $\mathbf{A}, \mathbf{B}, \mathbf{C}$ and $\mathbf{D}$ those matrices of respective dimensions $N' \times N'$, $N' \times n$, $n \times N'$ and $n \times n$ such that

$$\mathbf{Q}_{\mathcal{P},\mathbf{X}'}^{-1} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix}.$$

We have

$$\begin{pmatrix} \mathbf{K}_{\mathbf{X}'} & 0 \end{pmatrix} \mathbf{Q}_{\mathcal{P},\mathbf{X}'}^{-1} = \begin{pmatrix} \mathbf{K}_{\mathbf{X}'}\mathbf{A} & \mathbf{K}_{\mathbf{X}'}\mathbf{B} \end{pmatrix}.$$

Using $\mathbf{Q}_{\mathcal{P},\mathbf{X}'}\mathbf{Q}_{\mathcal{P},\mathbf{X}'}^{-1} = \mathrm{Id}_{N'+n}$, we get

$$\mathbf{K}_{\mathbf{X}'}\mathbf{A} = \mathrm{Id}_{N'} - \mathbf{P}_{\mathbf{X}'}\mathbf{C} \text{ and } \mathbf{K}_{\mathbf{X}'}\mathbf{B} = -\mathbf{P}_{\mathbf{X}'}\mathbf{D}$$

and eventually

$$\begin{pmatrix} \mathbf{K}_{\mathbf{X}'} & 0 \end{pmatrix} \mathbf{Q}_{\mathcal{P},\mathbf{X}'}^{-1} = \begin{pmatrix} \mathrm{Id}_{N'} & 0 \end{pmatrix} - \mathbf{P}_{\mathbf{X}'} \begin{pmatrix} \mathbf{C} & \mathbf{D} \end{pmatrix}.$$

3. Kriging ([4],[7]) is very popular in computer experiments and geostatistics. Let us recall how that technique is linked to interpolation. Kriging aims at approximating a function $f \in \mathbb{R}^E$ only known on a *design* $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset E$. In its simplest form, it postulates that f is a realization of a gaussian process F whose parameter lies in E:

$$F(\mathbf{x}) = \sum_{i=1}^{n} \beta_i p_i(\mathbf{x}) + Z(\mathbf{x}) \tag{5.17}$$

where $(p_1, \ldots, p_n)$ is a basis of a vector space of functions $\mathbb{P} \subset \mathbb{R}^E$ and Z is a centered gaussian process. Then it consists in approximating $f(\mathbf{x})$ by the best linear unbiased predictor (BLUP).
Now, it is readily seen that the BLUP depends on F only through this centered gaussian process whose parameter is in $\mathcal{M}_{\mathbb{P}}$:
$F_{\mathbb{P}}(\sum_{m=1}^{M} \mu_m \delta_{\mathbf{x}_k}) = \sum_{m=1}^{M} \mu_m F(\mathbf{x}_i)$.
Hence the idea of *intrinsic* kriging: forget the model (5.17) and start, instead, with G, a centered gaussian process whose parameter is in $\mathcal{M}_{\mathbb{P}}$ and whose covariance is specified by a $\mathbb{P}$-conditionally positive definite kernel K, then solve the BLUP equations with G in place of $F_{\mathbb{P}}$.
This method leads exactly to the same equations than those that are to be solved to get the interpolator $S_{K,\mathbb{P},\mathbf{X}}(f)$.

4. Observing that $\delta_{\mathbf{x}} - \sum_{k=1}^{N'} u_k(\mathbf{x}) \delta_{\mathbf{x}'_k} \in \mathcal{M}_{\mathbb{P}}$ we rediscover this error estimation

$$\begin{aligned} |f(\mathbf{x}) - S_{K,\mathbb{P},\mathbf{X}}(f)(\mathbf{x})| &= | \left[\delta_{\mathbf{x}} - \sum_{k=1}^{N'} u_k(\mathbf{x}) \delta_{\mathbf{x}'_k} \right] (f)| \\ &= | < F_K(\delta_{\mathbf{x}} - \sum_{k=1}^{N'} u_k(\mathbf{x}) \delta_{\mathbf{x}'_k}), f >_{\mathcal{H}_{K,\mathbb{P}}} \\ &= | < K_{\mathbf{x}} - \sum_{k=1}^{N'} u_k(\mathbf{x}) K_{\mathbf{x}'_k}, f >_{\mathcal{H}_{K,\mathbb{P}}} | \\ &\leq ||f||_{\mathcal{H}_{K,\mathbb{P}}} \; ||K_{\mathbf{x}} - \sum_{k=1}^{N'} u_k(\mathbf{x}) K_{\mathbf{x}'_k}||_{\mathcal{H}_{K,\mathbb{P}}}. \end{aligned}$$

6 Regularized regression in R.K.S.H.S

As in the previous section, it is assumed that $\mathbb{P}$ denotes a finite dimensional vector space of functions and that K is a $\mathbb{P}$-conditionally positive definite kernel. Furthermore, suppose that, besides the "design" $\mathbf{X}$, we are given values $\mathbf{y}_1, \ldots, \mathbf{y}_N \in \mathbb{R}$. For $\mathbb{P}$ a finite dimensional vector space and K a $\mathbb{P}$-conditionally positive definite kernel, we want now to solve the following regularized regression problem:

$$\min_{f \in \mathcal{H}_{K,\mathbb{P}}} \sum_{k=1}^{N} (\mathbf{y}_k - f(\mathbf{x}_k))^2 + \lambda ||f||^2_{\mathcal{H}_{K,\mathbb{P}}} \tag{6.1}$$

where λ is a strictly positive real.
The representer theorem is true in $\mathbb{P}$-R.K.S.H.S :

Theorem 6.1 *Any solution of (6.1) lies in* $\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X})$.

Proof
Let $f \in \mathcal{H}_{K,\mathbb{P}}$ be a solution of problem (6.1).
By Proposition 5.2, $g = S_{K,\mathbb{P},\mathbf{X}}(f)$ belongs to $\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X})$ and interpolates f on $\mathbf{X}$, hence

$$\sum_{k=1}^{N} (\mathbf{y}_k - f(\mathbf{x}_k))^2 = \sum_{k=1}^{N} (\mathbf{y}_k - g(\mathbf{x}_k))^2 \,.$$

Moreover, if f and g were distinct, the same proposition 5.2 would imply:

$$||g||_{\mathcal{H}_{K,\mathbb{P}}} < ||f||_{\mathcal{H}_{K,\mathbb{P}}}$$

so

$$\sum_{k=1}^{N}(\mathbf{y}_k - g(\mathbf{x}_k))^2 + \lambda||g||^2_{\mathcal{H}_{K,\mathbb{P}}} < \sum_{k=1}^{N}(\mathbf{y}_k - f(\mathbf{x}_k))^2 + \lambda||f||^2_{\mathcal{H}_{K,\mathbb{P}}}$$

which contradicts the fact that f is a solution of (6.1).
□
Explicit solution of (6.1) is given by:

Proposition 6.1 *Let* $\mathbf{X}$ *be a free* $\mathbb{P}$*-unisolvent set.*

The solution of (6.1) is $f = \sum_{i=1}^{n}\alpha_i p_i + \sum_{j=1}^{N}\gamma_j K_{\mathbf{x}_j}$ *with* $\boldsymbol{\alpha} = \begin{pmatrix}\alpha_1\\ \vdots \\ \alpha_n\end{pmatrix} \in \mathbb{R}^n, \boldsymbol{\gamma} = \begin{pmatrix}\gamma_1\\ \vdots \\ \gamma_M\end{pmatrix} \in \mathbb{R}^N$ *given by*

$$\left\{\begin{array}{l}\boldsymbol{\gamma} = (\mathbf{K_X} + \boldsymbol{\lambda}\mathrm{Id}_N)^{-1}(\mathbf{Y} - \mathbf{P_X}\boldsymbol{\alpha})\\ \boldsymbol{\alpha} = \left[\mathbf{P_X}^T(\mathbf{K_X} + \boldsymbol{\lambda}\mathrm{Id}_N)^{-1}\mathbf{P_X}\right]^{-1}\mathbf{P_X}^T(\mathbf{K_X} + \boldsymbol{\lambda}\mathrm{Id}_N)^{-1}\mathbf{Y}\end{array}\right. \tag{6.2}$$

where $\mathbf{Y} = \begin{pmatrix}y_1\\ \vdots \\ y_N\end{pmatrix}$.

Proof
From Theorem 6.1, we know that the solution is to be searched in $\mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X})$. The function $g = \sum_{i=1}^{n}\alpha_i^{(0)}p_i + \sum_{j=1}^{N}\gamma_j^{(0)}K_{\mathbf{x}_j} \in \mathbb{P} + \mathcal{F}_{K,\mathbb{P}}(\mathbf{X})$ is solution of (6.1) if and only if $\boldsymbol{\alpha}^{(0)} = \begin{pmatrix}\alpha_1^{(0)}\\ \vdots \\ \alpha_n^{(0)}\end{pmatrix} \in \mathbb{R}^n, \boldsymbol{\gamma}^{(0)} = \begin{pmatrix}\gamma_1^{(0)}\\ \vdots \\ \gamma_M^{(0)}\end{pmatrix} \in \mathbb{R}^N$ is solution of

$$\min\{J(\boldsymbol{\alpha},\boldsymbol{\gamma}) : \boldsymbol{\alpha} \in \mathbb{R}^n, \boldsymbol{\gamma} \in \mathbb{R}^N, \mathbf{P_X}^T\boldsymbol{\gamma} = 0\} \tag{6.3}$$

where

$$J(\boldsymbol{\alpha},\boldsymbol{\gamma}) = ||\mathbf{Y} - (\mathbf{K_X}\boldsymbol{\gamma} + \mathbf{P_X}\boldsymbol{\alpha})||^2_{\mathbb{R}^N} + \lambda\boldsymbol{\gamma}^T\mathbf{K_X}\boldsymbol{\gamma}\,.$$

To solve (6.3) let us form the Lagrangian

$$L(\boldsymbol{\alpha},\boldsymbol{\gamma},\boldsymbol{\mu}) = J(\boldsymbol{\alpha},\boldsymbol{\gamma}) + <\mathbf{P_X}^T, \boldsymbol{\mu}>_{\mathbb{R}^n}\ .$$

A solution of (6.3) satisfies the following first order conditions:

$$\left\{\begin{array}{l}2\mathbf{P_X}^T\left[\mathbf{K_X}\boldsymbol{\gamma} + \mathbf{P_X}\boldsymbol{\alpha} - \mathbf{Y}\right] = 0\\ 2\mathbf{K_X}\left[\mathbf{K_X}\boldsymbol{\gamma} + \mathbf{P_X}\boldsymbol{\alpha} - \mathbf{Y}\right] + 2\boldsymbol{\lambda}\mathbf{K_X}\boldsymbol{\gamma} + \mathbf{P_X}\boldsymbol{\mu} = 0\\ \mathbf{P_X}^T\boldsymbol{\gamma} = 0\end{array}\right. . \tag{6.4}$$

Rewriting first equation as $\left\{\begin{array}{l}\mathbf{K_X}\boldsymbol{\gamma} + \mathbf{P_X}\boldsymbol{\alpha} - \mathbf{Y} = \mathbf{e}\\ \mathbf{P_X}^T\mathbf{e} = 0\end{array}\right.$, (6.4) becomes

$$\left\{\begin{array}{l}\mathbf{K_X}\boldsymbol{\gamma} + \mathbf{P_X}\boldsymbol{\alpha} - \mathbf{Y} = \mathbf{e}\\ \mathbf{K_X}\left[\mathbf{e} + \boldsymbol{\lambda}\boldsymbol{\gamma}\right] + \mathbf{P_X}(\tfrac{1}{2}\boldsymbol{\mu}) = 0\\ \mathbf{P_X}^T\mathbf{e} = 0\\ \mathbf{P_X}^T\boldsymbol{\gamma} = 0\end{array}\right. . \tag{6.5}$$

From the three last equations we then draw:

$$\left\{\begin{array}{l}\mathbf{K}_\mathbf{X}\left[\mathbf{e}+\boldsymbol{\lambda}\boldsymbol{\gamma}\right]+\mathbf{P}_\mathbf{X}(\frac{1}{2}\boldsymbol{\mu})=0\\ {\mathbf{P}_\mathbf{X}}^T\left[\mathbf{e}+\boldsymbol{\lambda}\boldsymbol{\gamma}\right]=0\end{array}\right. . \tag{6.6}$$

Since $\mathbf{X}$ is free, Lemma 5.3 implies that $\begin{pmatrix}\mathbf{K}_\mathbf{X} & \mathbf{P}_\mathbf{X}\\ {\mathbf{P}_\mathbf{X}}^T & 0\end{pmatrix}$ is non degenerate. Hence (6.6) gives

$$\left\{\begin{array}{l}\mathbf{e}+\boldsymbol{\lambda}\boldsymbol{\gamma}=0\\ \boldsymbol{\mu}=0\end{array}\right. \Rightarrow \left\{\begin{array}{l}\mathbf{e}=-\boldsymbol{\lambda}\boldsymbol{\gamma}\\ \boldsymbol{\mu}=0\end{array}\right.$$

and, used in (6.5)

$$\left\{\begin{array}{l}\boldsymbol{\gamma}=(\mathbf{K}_\mathbf{X}+\boldsymbol{\lambda}\mathrm{Id}_N)^{-1}(\mathbf{Y}-\mathbf{P}_\mathbf{X}\boldsymbol{\alpha})\\ {\mathbf{P}_\mathbf{X}}^T(\mathbf{K}_\mathbf{X}+\boldsymbol{\lambda}\mathrm{Id}_N)^{-1}\mathbf{P}_\mathbf{X}\boldsymbol{\alpha}={\mathbf{P}_\mathbf{X}}^T(\mathbf{K}_\mathbf{X}+\boldsymbol{\lambda}\mathrm{Id}_N)^{-1}\mathbf{Y}\end{array}\right. . \tag{6.7}$$

Notice, then, that ${\mathbf{P}_\mathbf{X}}^T(\mathbf{K}_\mathbf{X}+\boldsymbol{\lambda}\mathrm{Id}_N)^{-1}\mathbf{P}_\mathbf{X}$ is a symmetric positive definite matrix. Indeed, $(\mathbf{K}_\mathbf{X}+\boldsymbol{\lambda}\mathrm{Id}_N)^{-1}$ is obviously a symmetric positive definite matrix so that

$$\mathbf{a}^T{\mathbf{P}_\mathbf{X}}^T(\mathbf{K}_\mathbf{X}+\boldsymbol{\lambda}\mathrm{Id}_N)^{-1}\mathbf{P}_\mathbf{X}\mathbf{a}=0 \Leftrightarrow \mathbf{P}_\mathbf{X}\mathbf{a}=0$$

which implies $\mathbf{a}=0$ since $\mathbf{X}$ is $\mathbb{P}$-unisolvent.
Hence, eventually, (6.7) leads to

$$\left\{\begin{array}{l}\boldsymbol{\gamma}=(\mathbf{K}_\mathbf{X}+\boldsymbol{\lambda}\mathrm{Id}_N)^{-1}(\mathbf{Y}-\mathbf{P}_\mathbf{X}\boldsymbol{\alpha})\\ \boldsymbol{\alpha}=\left[{\mathbf{P}_\mathbf{X}}^T(\mathbf{K}_\mathbf{X}+\boldsymbol{\lambda}\mathrm{Id}_N)^{-1}\mathbf{P}_\mathbf{X}\right]^{-1}{\mathbf{P}_\mathbf{X}}^T(\mathbf{K}_\mathbf{X}+\boldsymbol{\lambda}\mathrm{Id}_N)^{-1}\mathbf{Y}\end{array}\right. .$$

□

The solution (6.2) is formally the same as the one proposed by G. Wahba [9] in the context of thin-plate splines on $\mathbb{R}^d$ which is known to correspond to this $\mathbb{P}$-conditionally positive definite kernel:

$$K(\mathbf{x},\mathbf{x}')=(-1)^{k+1}||\mathbf{x}-\mathbf{x}'||_{\mathbb{R}^d}^{2k}\log(||\mathbf{x}-\mathbf{x}'||_{\mathbb{R}^d})$$

where $\mathbb{P}$ is the set of the d-variate polynomials of degree less than $k+1$.

7 Discussion

In this paper we propose a new definition of the *conditionally positive definite kernel* which, generalizing the usual one, leads to a full extension of the results of the positive definite case.
The core of our work is an Aronszajn's theorem analog which links any conditionally positive definite kernel to a functional semi-Hilbert space (R.K.S.H.S), generalizing R.K.H.S for positive definite kernel.
We show that the useful interpolation operator still works and specifically can be computed in this generalized context. As an other benchmark test we state the explicit solution of a regularized regression problem, which we recognize to be formally identical to the one stated in [9], in the context of thin-plate splines.

Contents

References

[1] N. Aronszajn. Theory of reproducing kernel. *Transactions of American Mathematical Society*, 68(3):337–404, 1950.

[2] N. Cressie. *Statistics for spatial data.* Wiley & Sons, New-York, 1993.

[3] G. Kimeldorf and G. Wahba. Some results on tchebycheffian spline functions. *Journal of Mathematical Analysis and Applications*, 33(1):82–95, 1971.

[4] J. R. Koehler and A. B. Owen. Computer experiments. In *Design and analysis of experiments*, volume 13 of *Handbook of Statist.*, pages 261–308. North-Holland, Amsterdam, 1996.

[5] R. Schaback. Native Hilbert spaces for radial basis functions. I. In *New developments in approximation theory (Dortmund, 1998)*, volume 132 of *Internat. Ser. Numer. Math.*, pages 255–282. Birkhäuser, Basel, 1999.

[6] R. Schaback. Kernel-based meshless methods. Technical report, Institute for Numerical and Applied Mathematics, Georg-August-University Goettingen, 2007.

[7] E. Vasquez. *Modélisation comportementale de systèmes non-linéaires multivariables par méthodes à noyaux et applications.* PhD thesis, Université Paris-sud, 2005.

[8] H. Wackernagel. *Multivariate Geostatistics: An Introduction with Applications.* Springer, 2003.

[9] G. Wahba. *Spline models for observational data*, volume 59 of *CBMS-NSF Regional Conference Series in Applied Mathematics.* Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 1990.

[10] H. Wendland. Spatial coupling in aeroelasticity by meshless kernel-based methods. In *ECCOMAS CFD 2006.*

[11] H. Wendland. *Scattered data approximation*, volume 17 of *Cambridge Monographs on Applied and Computational Mathematics.* Cambridge University Press, Cambridge, 2005.

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